

SUPPLEMENTARY INFORMATION

Utility of α -halodicyclopentadienones for the synthesis of novel fused heterocycles

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INN-SOHAN-185-1H

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PROCNO 1

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SOLVENT DMSO
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DS 2
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FIDRES 0.152588 Hz
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RG 30.72
DW 50.000 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
TDO 1

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NUC1 1H
P1 13.00 usec
PLW1 13.00000000 W

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LB 0.30 Hz
GB 0
PC 1.00

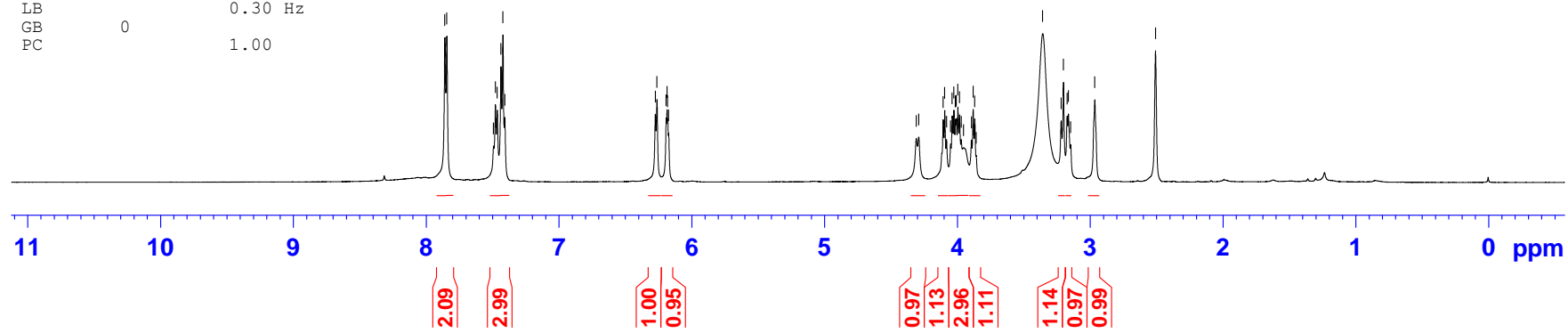


Figure S1. ¹H NMR of compound 3a

INN-TGL-04-54-13C

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NAME INN-TGL-04-54-13C
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PROCNO 1

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PROBHD Z163739_0226 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 5000
DS 0
SWH 27777.778 Hz
FIDRES 0.847710 Hz
AQ 1.1796480 sec
RG 101
DW 18.000 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6242384 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 97.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 25.07999992 W
PLW12 0.19815999 W
PLW13 0.09967500 W

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SSB 0
LB 1.00 Hz
GB 0
PC 1.40

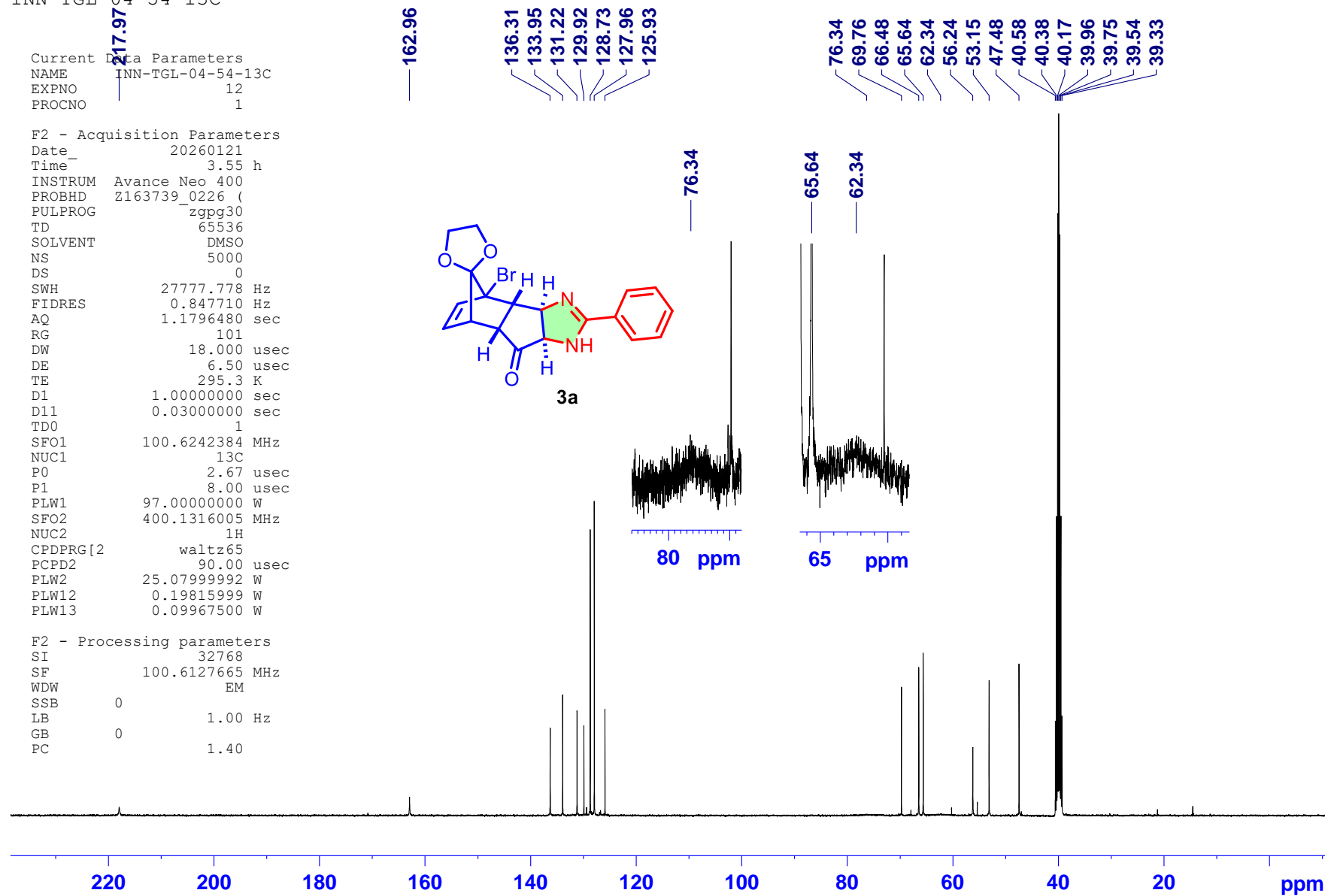


Figure S2. ¹³C NMR of compound 3a

INN-TGL-04-55-01-01-1H-WS

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EXPNO 7
PROCNO 1

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Time 20.00 h
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PROBHD z163739_0705 (
PULPROG zgpr
TD 51724
SOLVENT DMSO
NS 50
DS 4
SWH 11904.762 Hz
FIDRES 0.460319 Hz
AQ 2.1724081 sec
RG 101
DW 42.000 usec
DE 10.66 usec
TE 297.8 K
D1 1.00000000 sec
D12 0.00002000 sec
TD0 1
SFO1 400.3014394 MHz
NUC1 1H
P1 8.00 usec
PLW1 20.78400040 W
PLW9 0.00005321 W

F2 - Processing parameters
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SF 400.3000036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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7.751
7.633
7.612
6.258
6.242
6.165
6.156
6.141
4.297
4.273
4.082
4.068
4.052
4.029
4.014
3.998
3.987
3.974
3.959
3.945
3.876
3.859
3.845
3.161
2.946
2.502

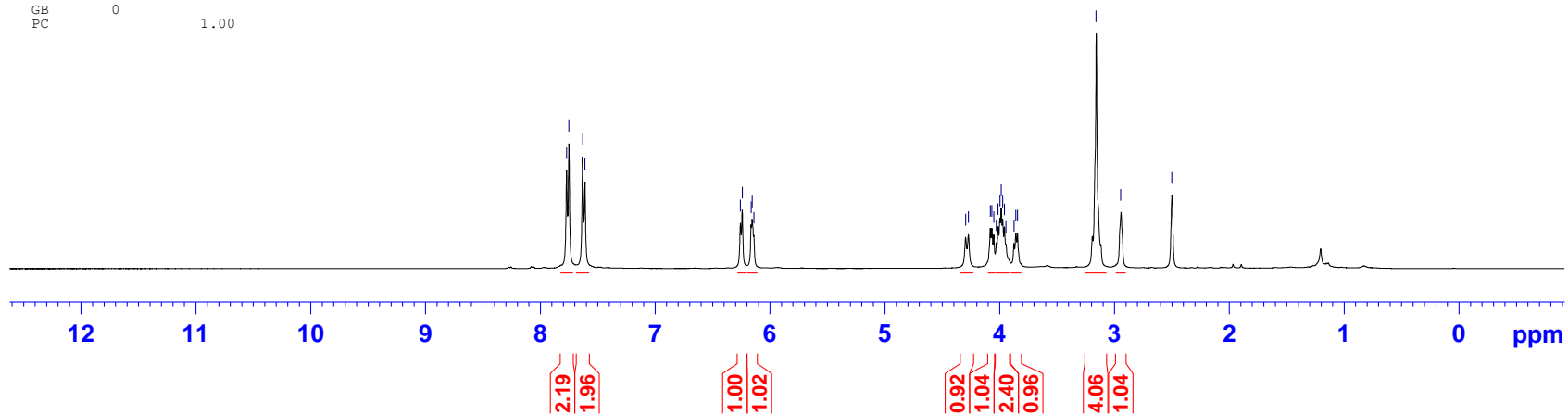
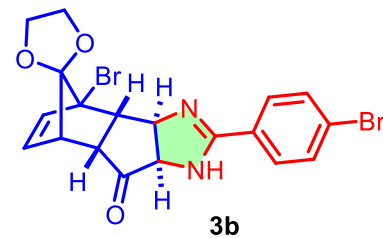


Figure S3. ¹H NMR of compound 3b

INN-TGL-04-55-01-13C

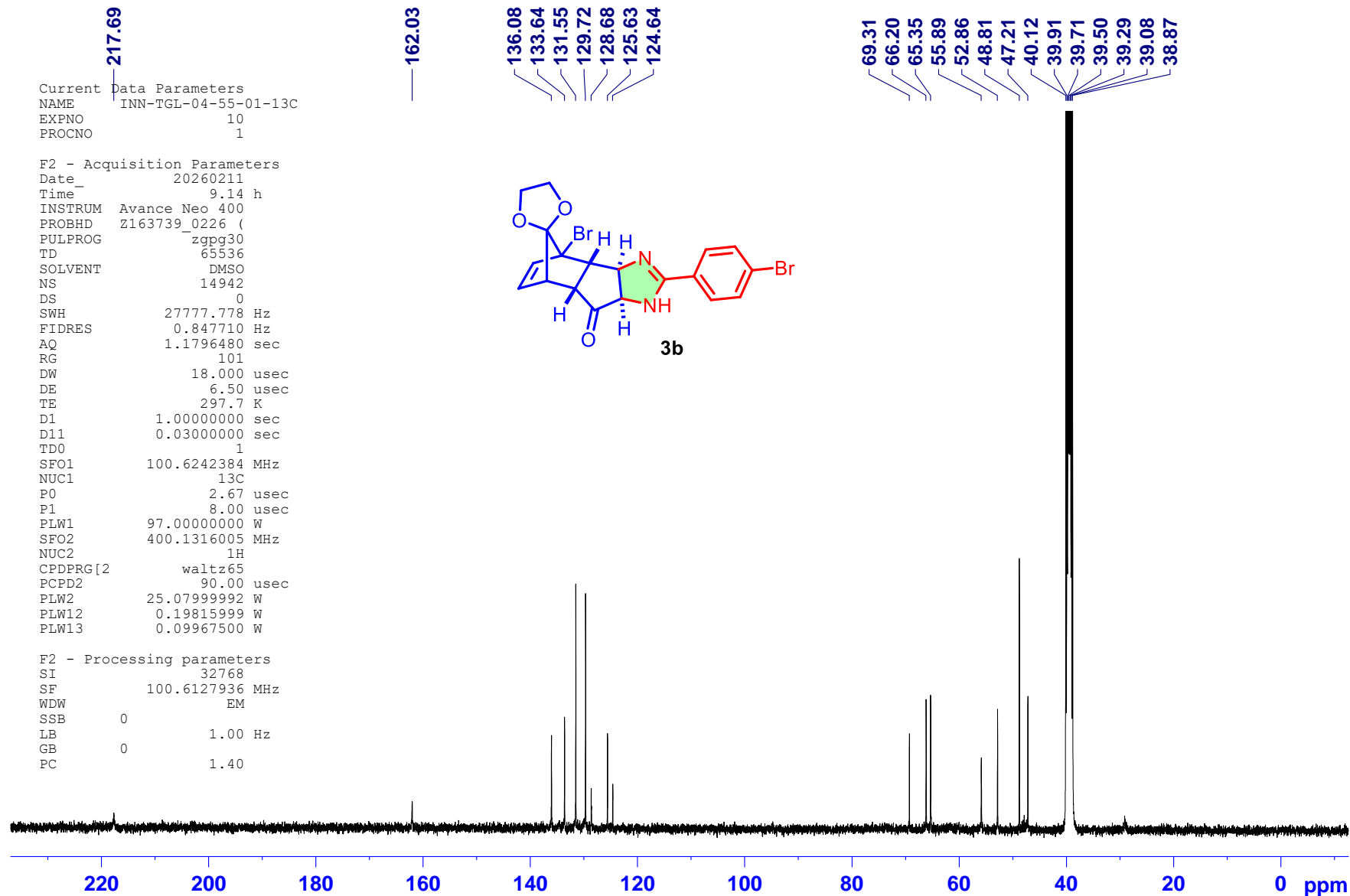


Figure S4. ¹³C NMR of compound 3b

INN-SOHAN-II-207-1H

Current Data Parameters
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EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171015
Time_ 0.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 81
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 48.36
DW 50.000 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 13.35 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

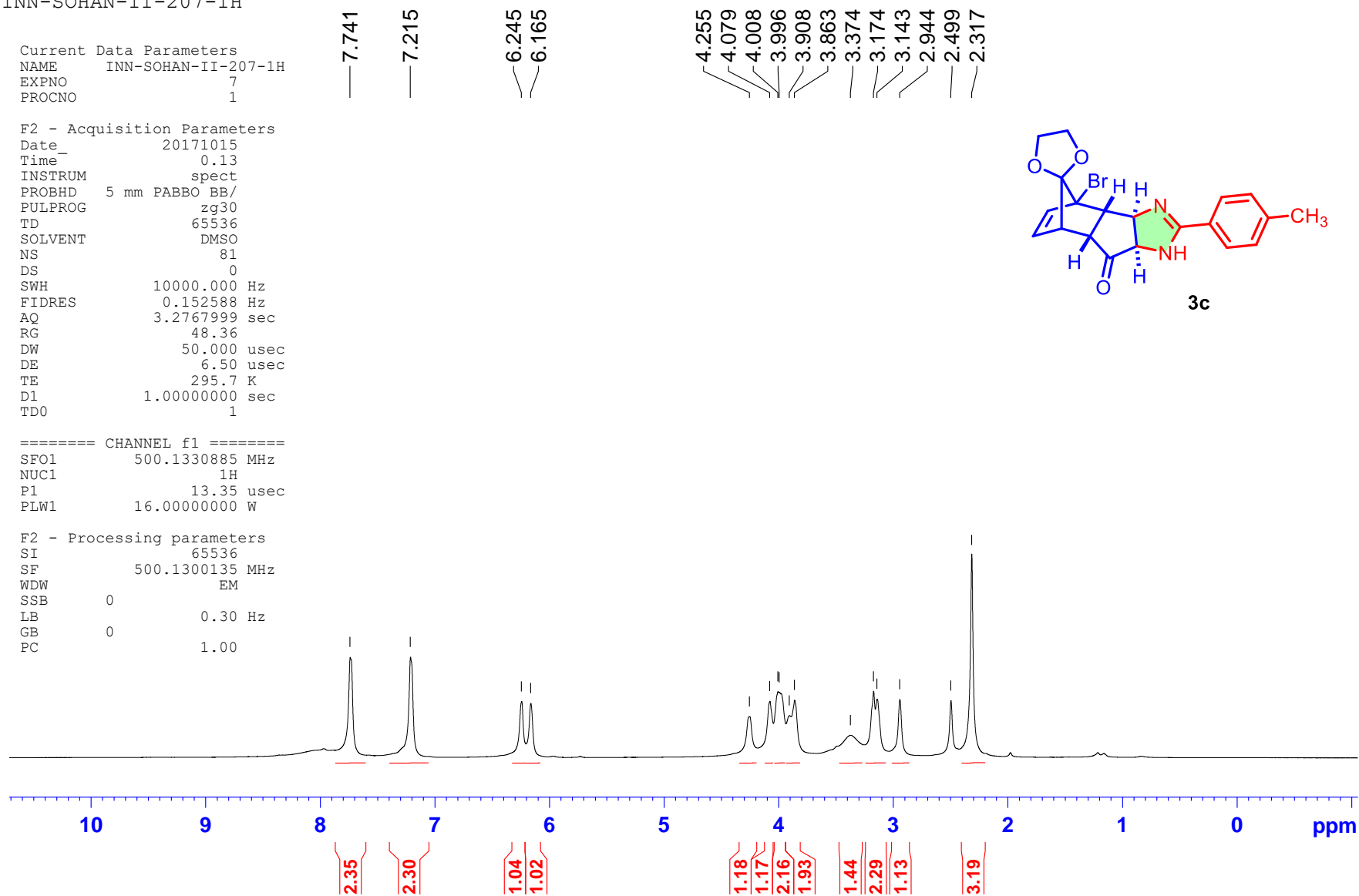


Figure S5. ¹H NMR of compound 3c

INN-SOHAN-II-207-13C

Current Data Parameters
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EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171015
Time_ 0.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15000
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 197.27
DW 15.000 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

=====
CHANNEL f1
SFO1 125.7716224 MHz
NUC1 13C
P1 8.90 usec
PLW1 103.0000000 W

=====
CHANNEL f2
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.44556001 W
PLW13 0.22411001 W

F2 - Processing parameters
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SF 125.7578508 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

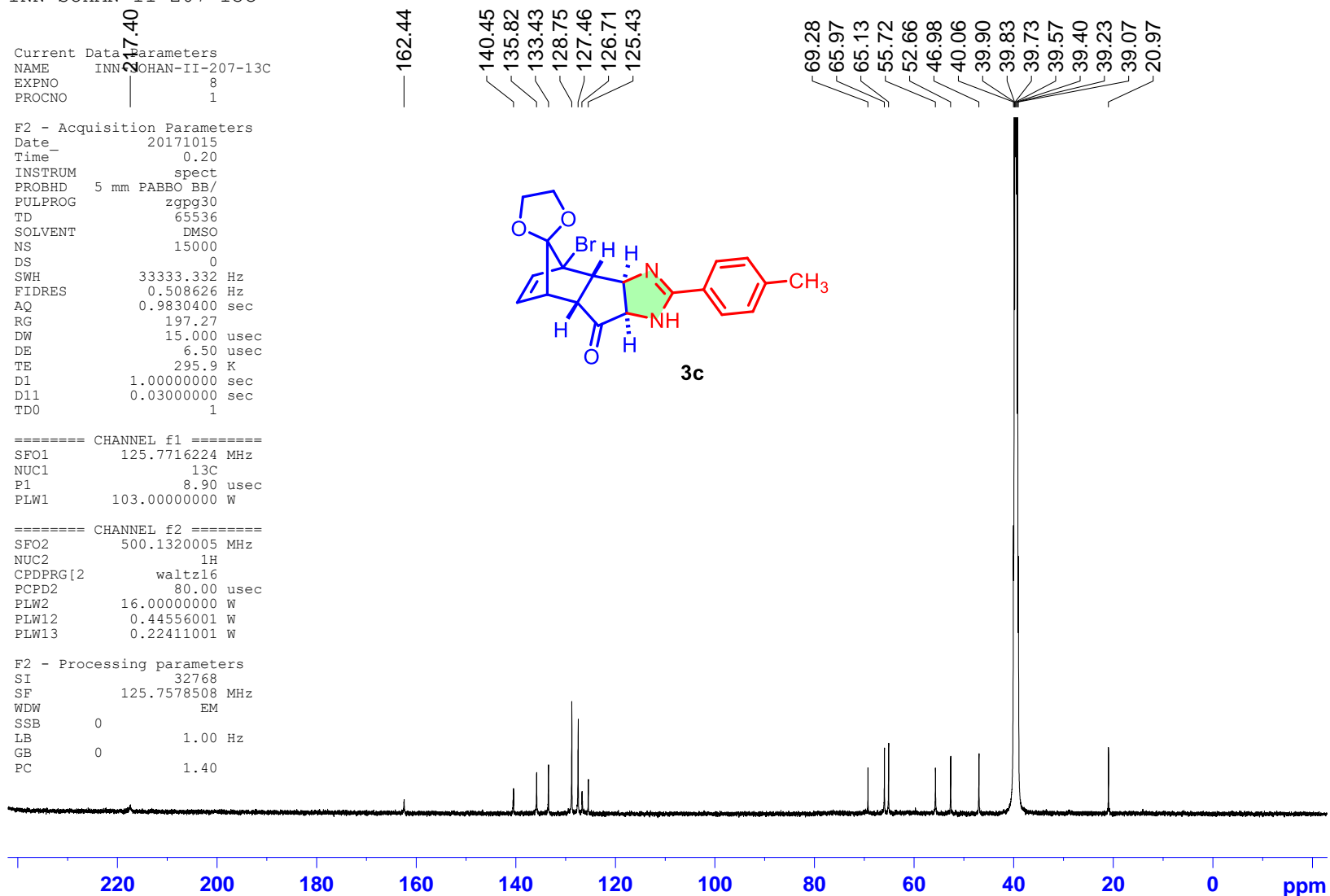


Figure S6. ¹³C NMR of compound 3c

INN-SOHAN-II-207-APT

Current Data Parameters
NAME INN-SOHAN-II-207-APT
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171015
Time 22.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 3602
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 197.27
DW 15.000 usec
DE 6.50 usec
TE 295.8 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
D20 0.00689655 sec
TD0 1

=====
CHANNEL f1
SFO1 125.7716224 MHz
NUC1 13C
P1 8.90 usec
P2 17.80 usec
PLW1 103.00000000 W

=====
CHANNEL f2
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.44556001 W

F2 - Processing parameters
SI 32768
SF 125.7578517 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

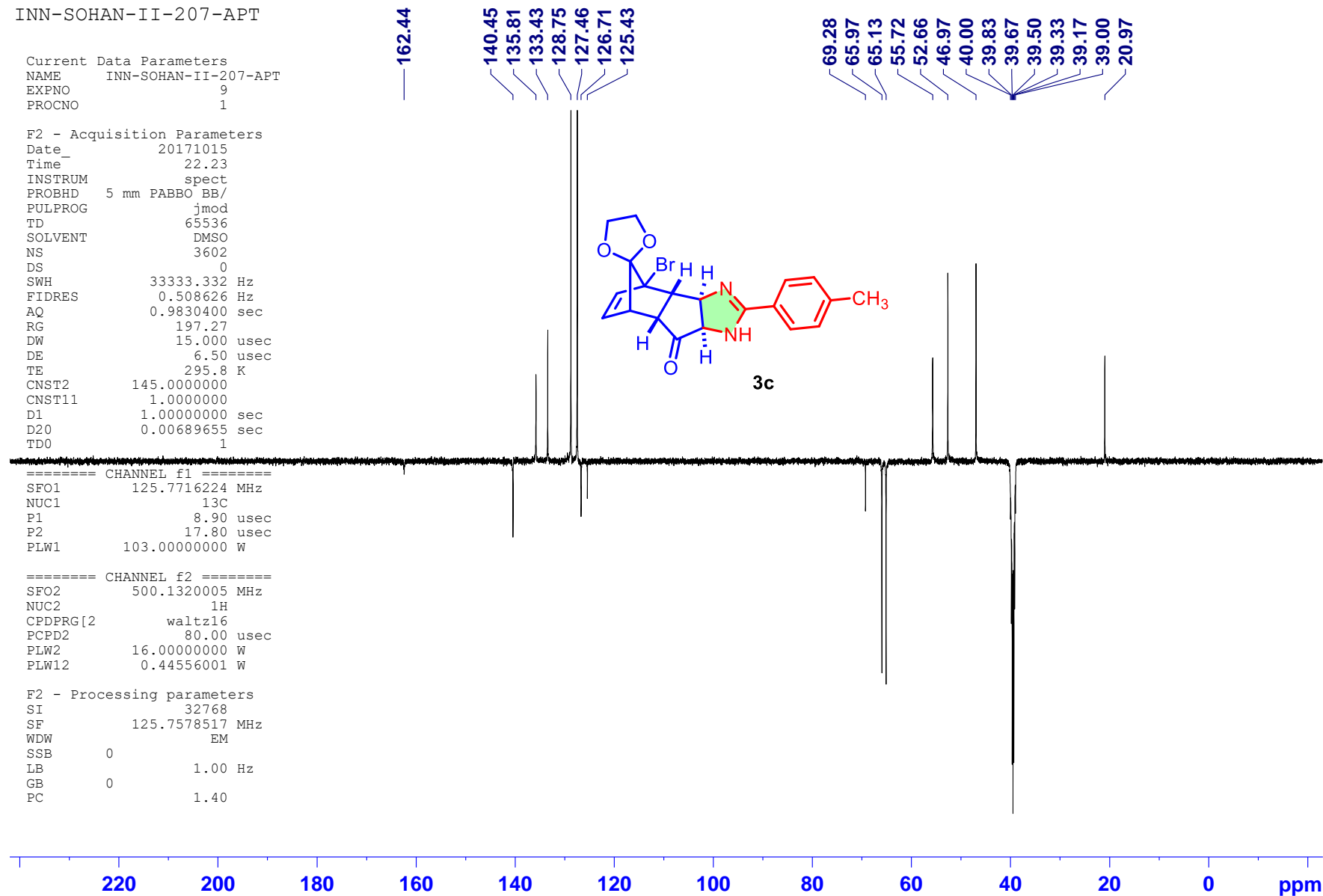


Figure S7. ¹³C-APT NMR of compound 3c

INN-SOHAN-II-29-1H

Current Data Parameters
NAME INN-SOHAN-II-29-1H
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180419
Time_ 21.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 30
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 30.72
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SF01 500.1330885 MHz
NUC1 1H
P1 13.35 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300150 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.729 7.714 7.421 7.407 7.393 7.356 7.340 7.325 7.260 6.245 6.128 6.123 6.118 5.262 4.263 4.244 3.747 3.729 3.233 3.199 3.191 3.182 3.174 2.975 2.965 2.958 2.949 1.567 1.550 1.470 1.453

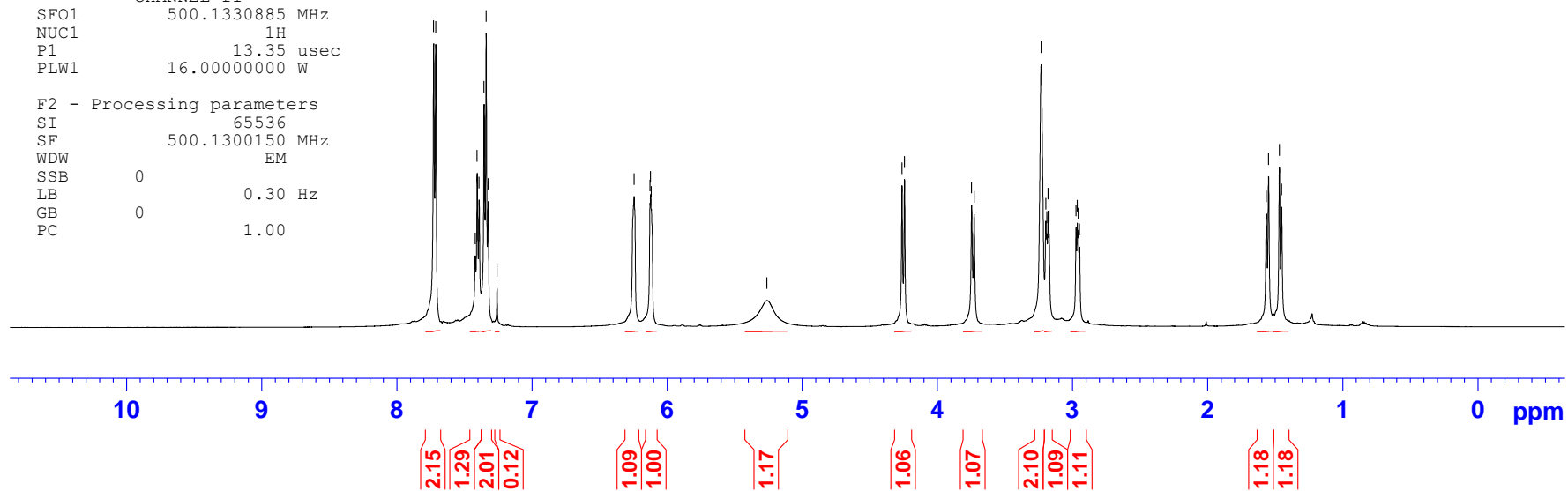
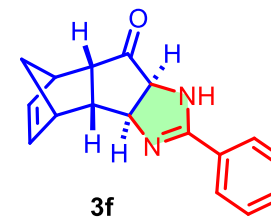


Figure S8. ¹H NMR of compound 3f

INN-SOHAN-II-29-13C

Current Data Parameters
NAME INN-SOHAN-II-29-13C
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180419
Time 21.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 578
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 197.27
DW 15.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 125.7716224 MHz
NUC1 13C
P1 8.90 usec
PLW1 103.00000000 W

----- CHANNEL f2 -----
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.44556001 W
PLW13 0.22411001 W

F2 - Processing parameters
SI 32768
SF 125.7577778 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB
PC 1.40

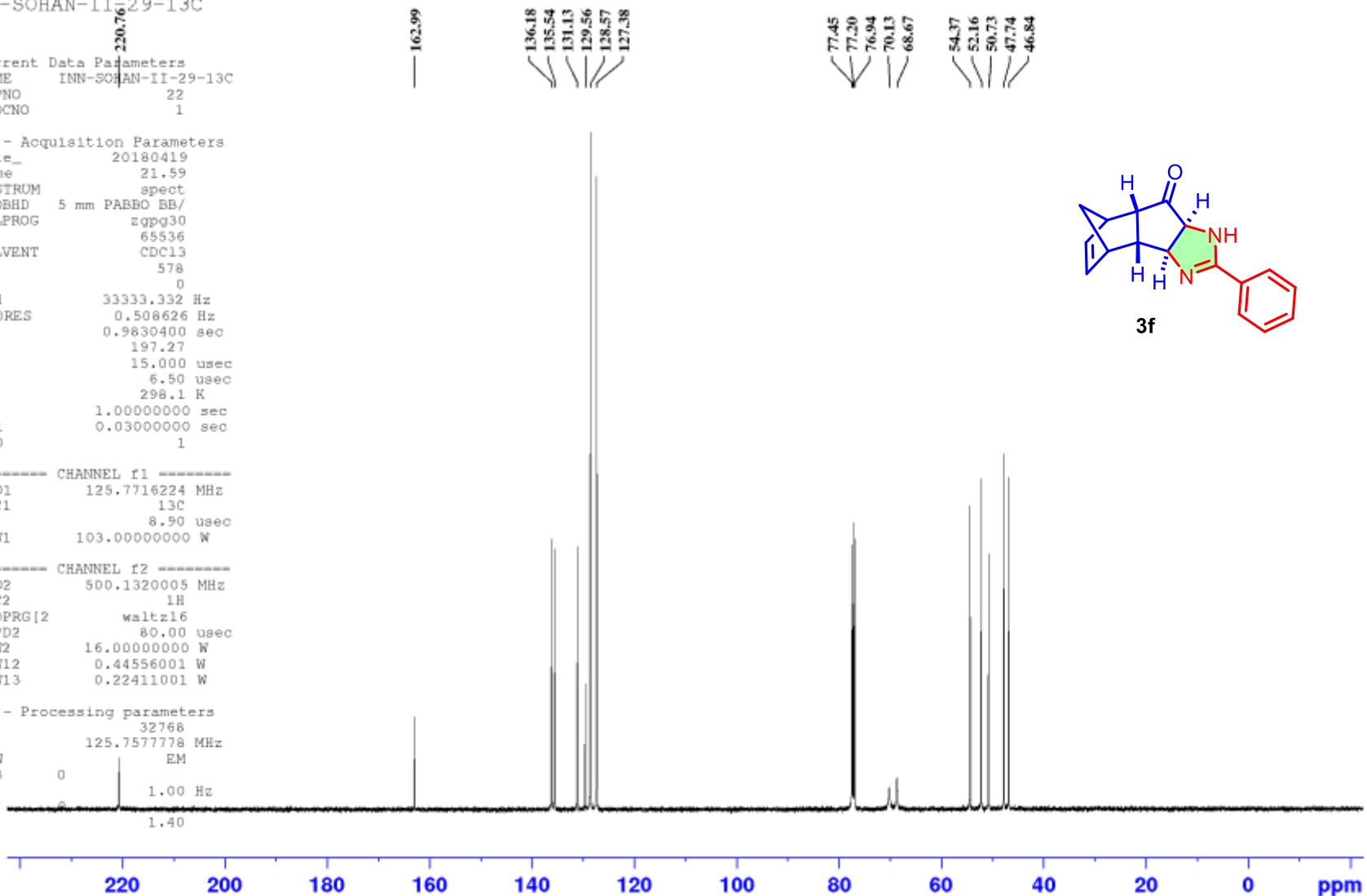


Figure S9. ¹³C NMR of compound 3f

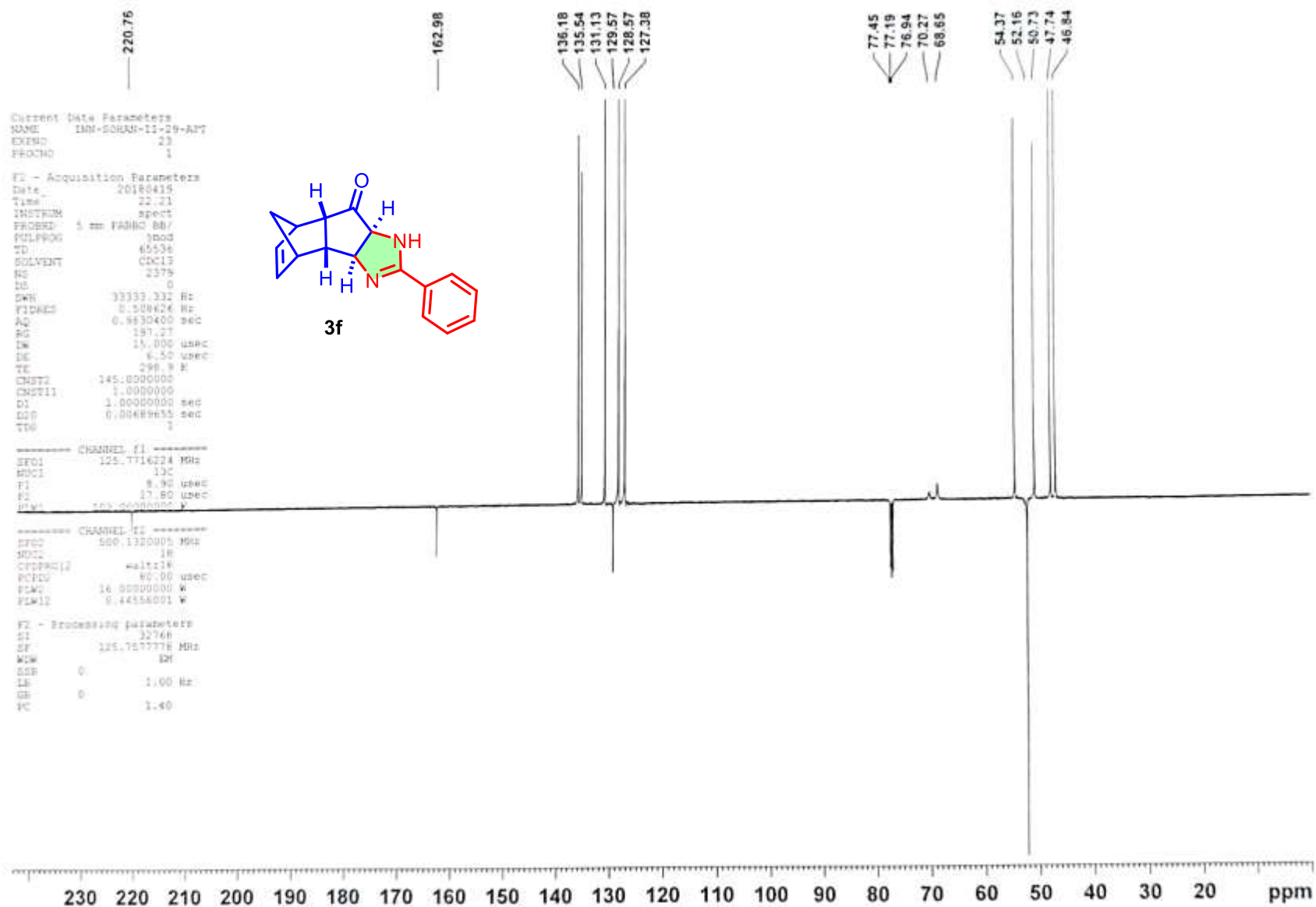


Figure S10. ¹³C-APT NMR of compound 3f

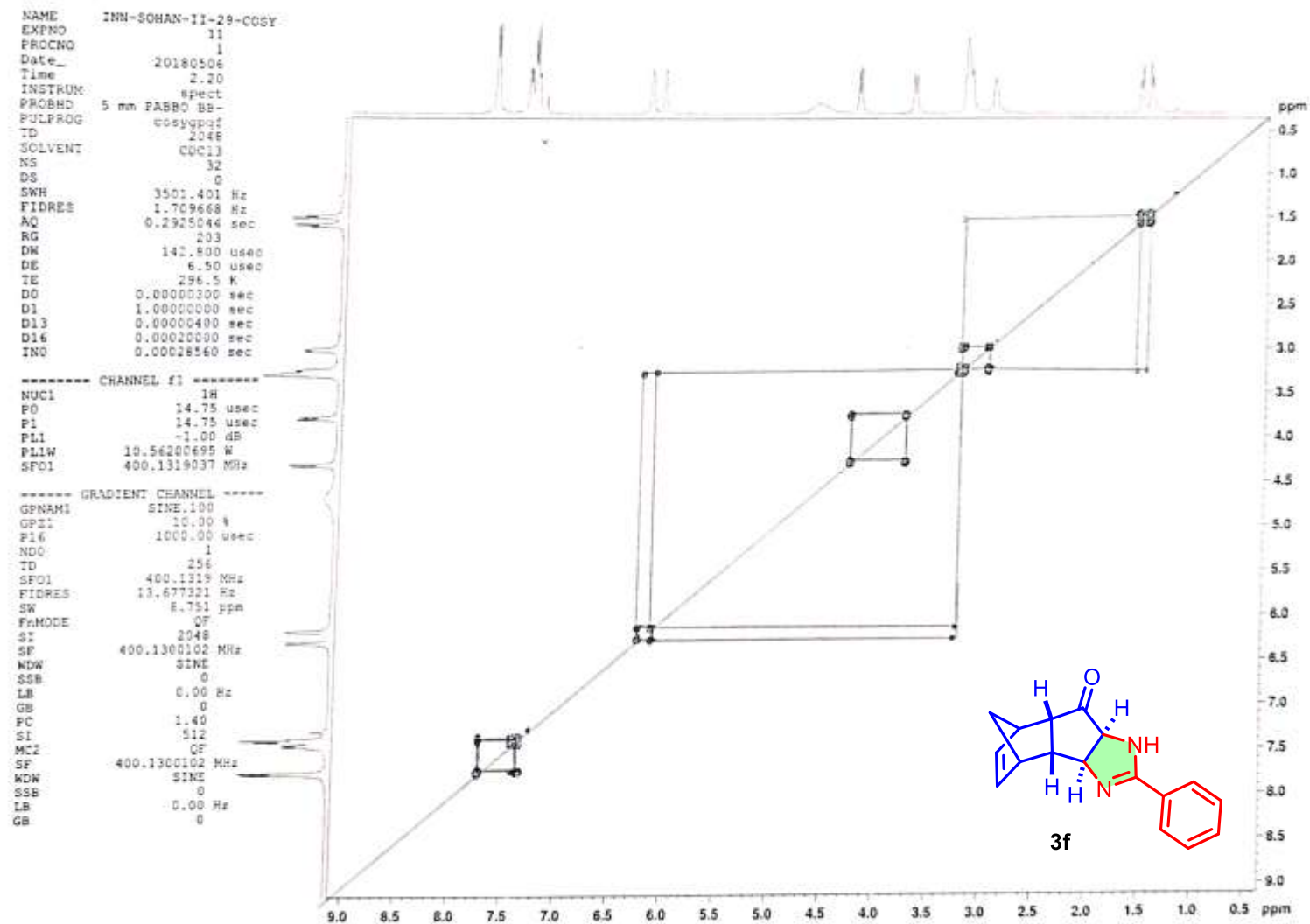


Figure S11. ^1H - ^1H COSY NMR of compound **3f**

```

Current Data Parameters
NAME      INN-SOHAN-185B-1H
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20151209
Time      10.54
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PROBHD    5 mm PABBO BB/
FULPROG   zg30
TD         65536
SOLVENT   Acetone
NS         38
DS         2
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2767999 sec
RG         61.42
DW         50.000 usec
DE         6.50 usec
TE         296.0 K
D1         1.00000000 sec
TDO        1

```

```

===== CHANNEL f1 =====
SFO1      500.1330885 MHz
NUC1       1H
P1         13.00 usec
PLW1       13.00000000 W

```

```

F2 - Processing parameters
SI         65536
SF         500.1300082 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00

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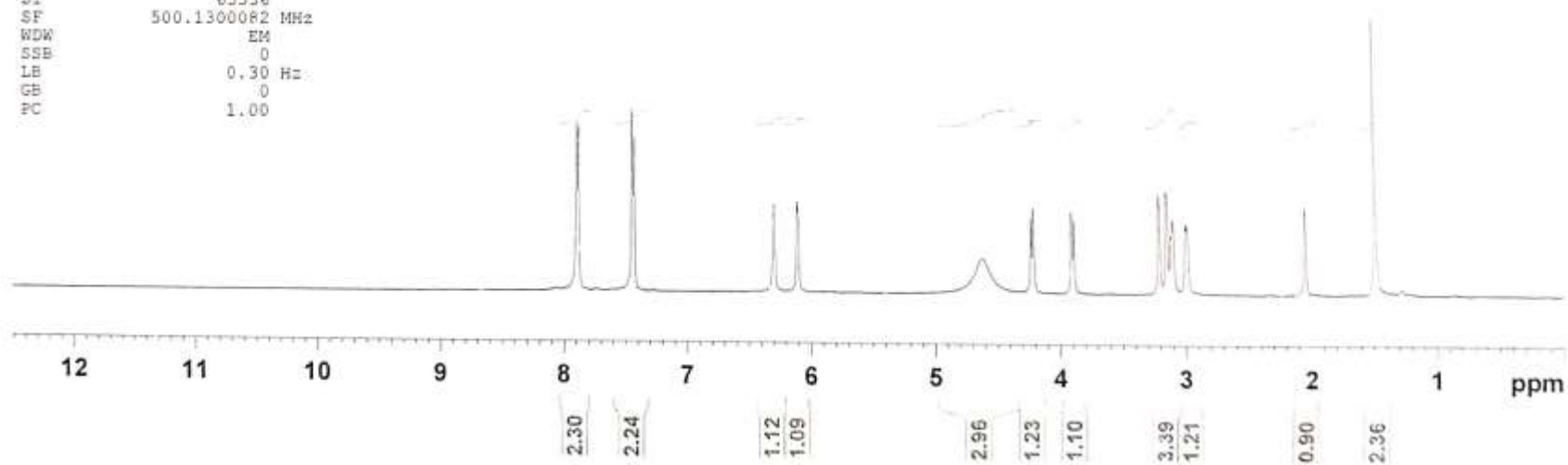
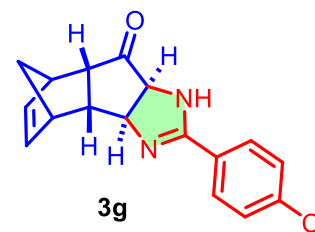


Figure S12. ¹H NMR of compound **3g**

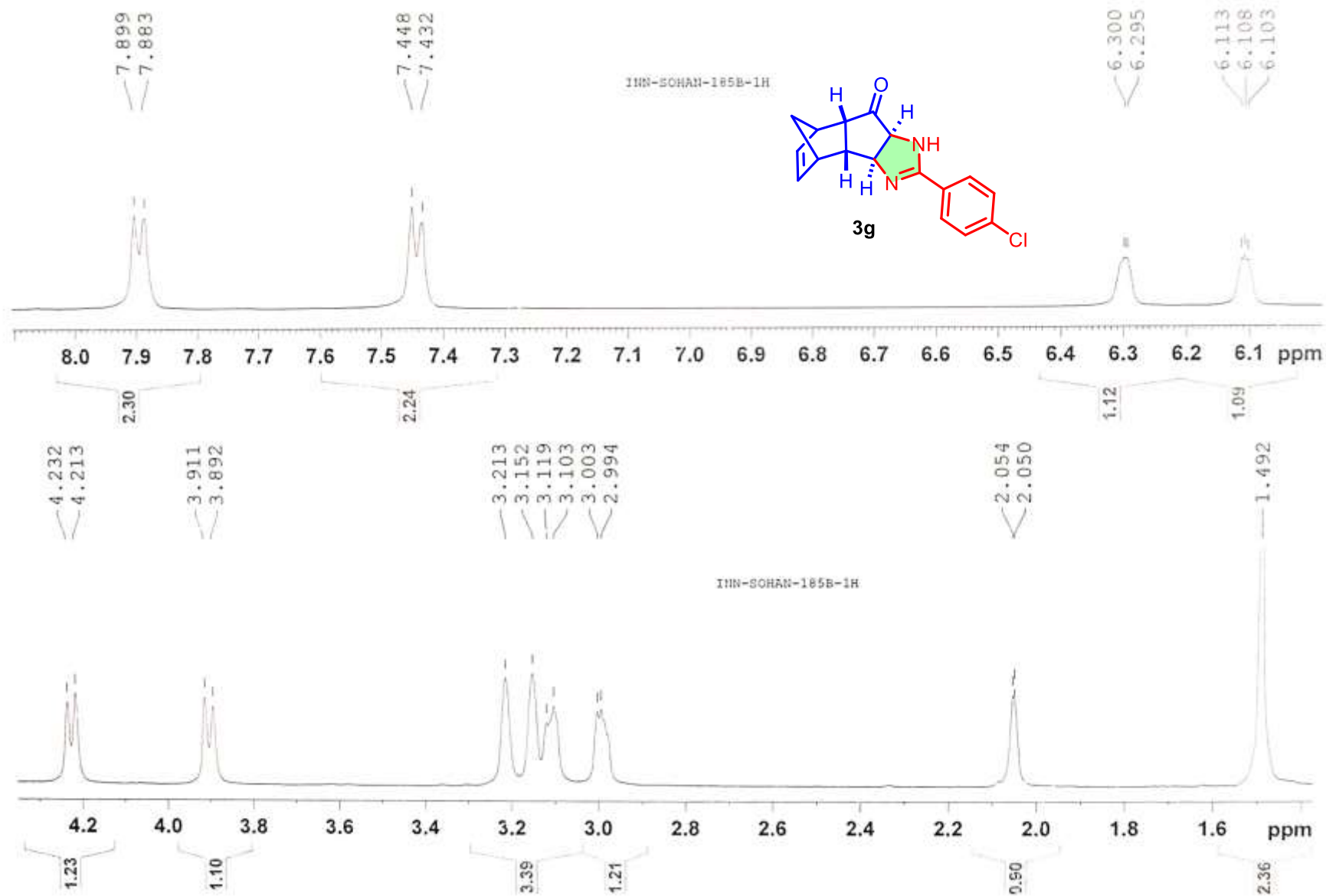


Figure S12a. ¹H NMR of compound 3g

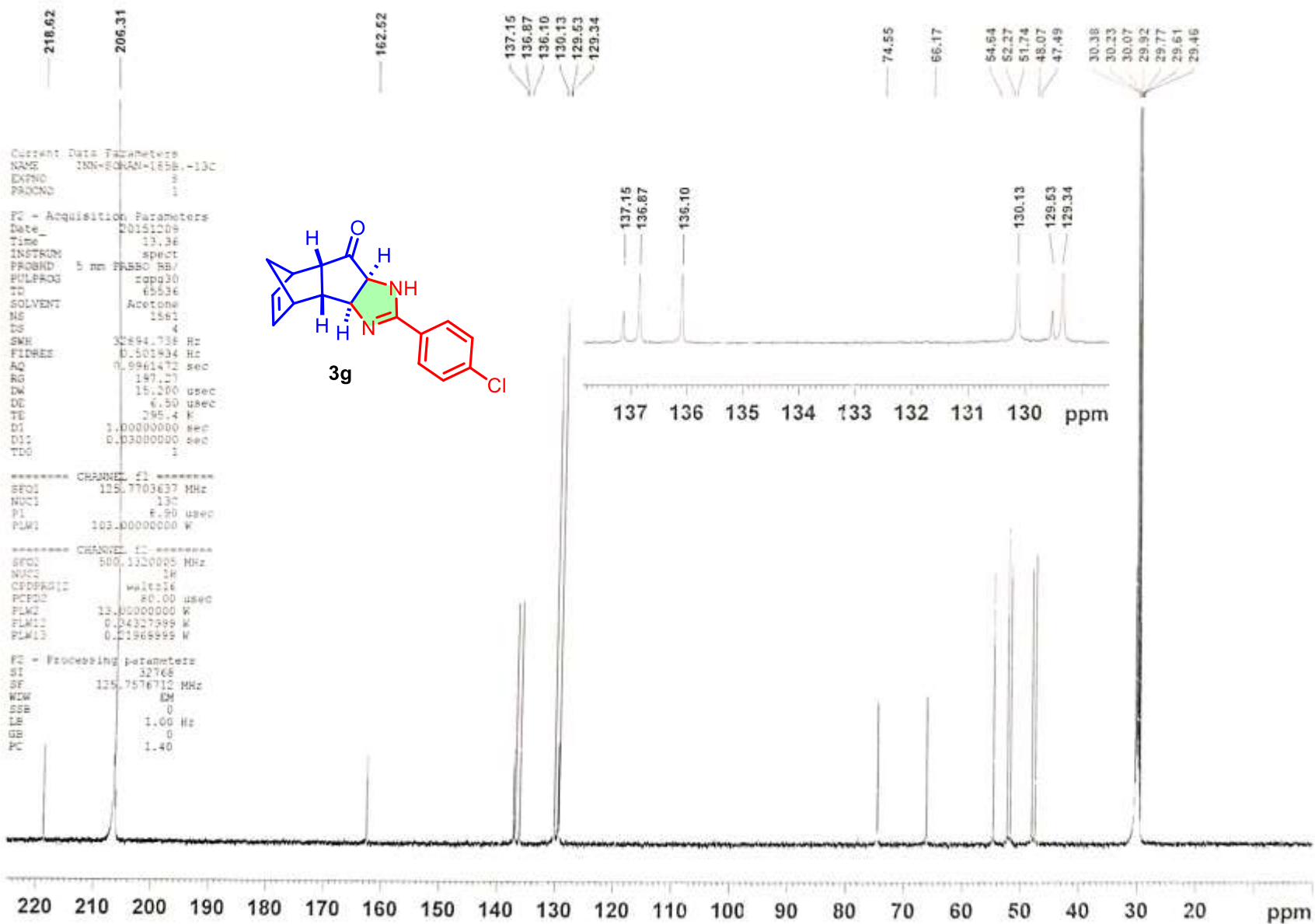


Figure S13. ¹³C NMR of compound 3g

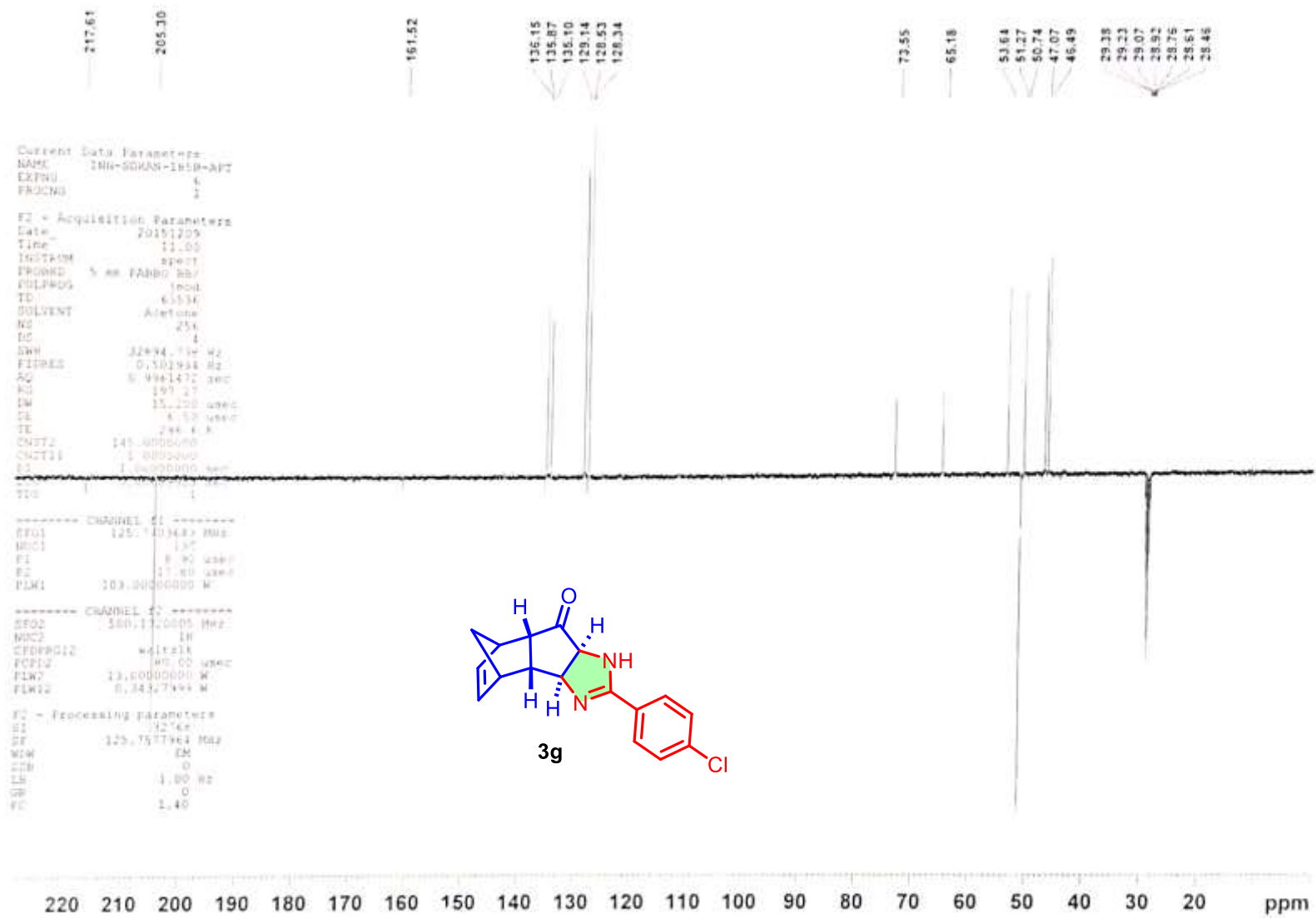


Figure S14. ¹³C-APT NMR of compound 3g

INN-SOHAN-II-369-1H

Current Data Parameters
NAME INN-SOHAN-II-369-1H
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180508
Time_ 1.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 60
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 30.72
DW 50.000 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 13.35 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0 0.30 Hz
GB 0
PC 1.00

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7.604
7.599
7.260
7.163
7.147
7.129
6.258
6.252
6.244
6.139
6.133
6.121
5.453

4.268
4.249
4.224
3.733
3.714
3.226
3.192
3.184
2.984
2.967
2.958
2.341
2.324
1.576
1.559
1.542
1.481
1.462
1.444

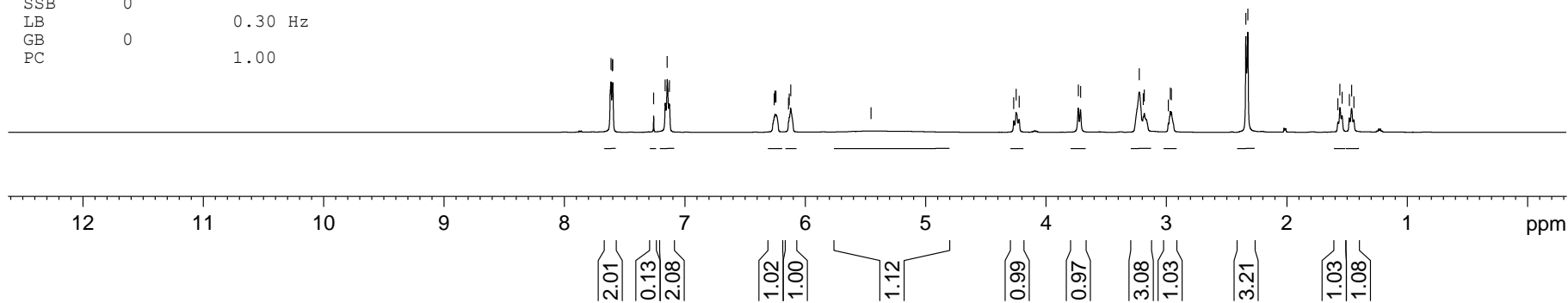
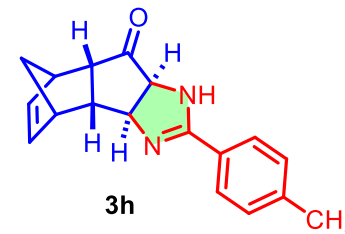


Figure S15. ¹H NMR of compound 3h

INN-SOHAN-II-369-13C

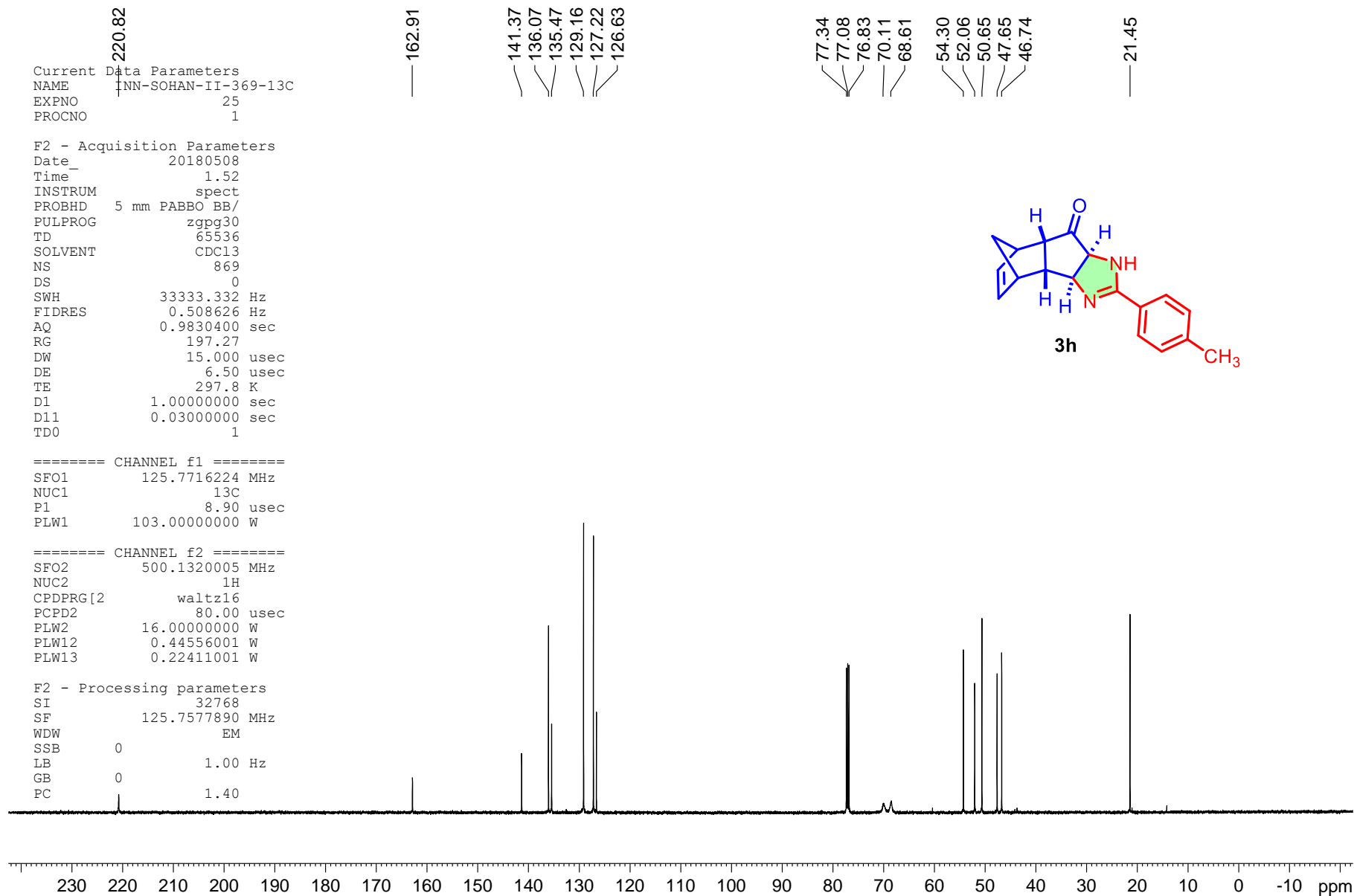


Figure S16. ¹³C NMR of compound 3h

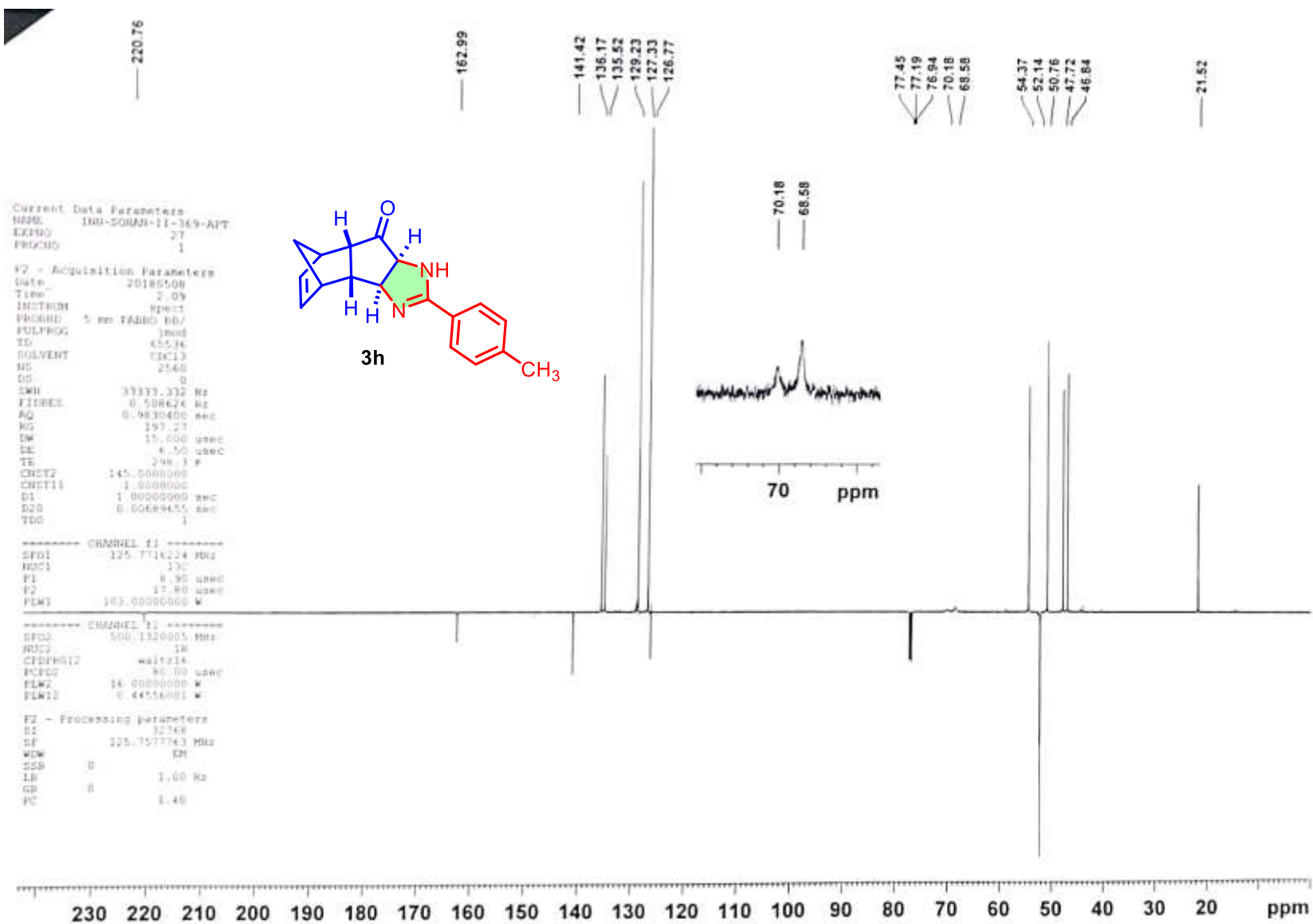


Figure S17. ^{13}C -APT NMR of compound **3h**

Current Data Parameters
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EXPNO 27
PROCNO 1

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Time_ 3.38
INSTRUM spect
PROBHD 5 mm F400 Ns/
PULPROG cosygpcpqf
TD 2048
SOLVENT CDC13
NS 24
DS 0
SWH 4302.926 Hz
FIDRES 2.101038 Hz
AQ 0.2379776 sec
RG 106.34
DN 116.200 usec
DE 6.50 usec
TE 299.2 K
D0 0.0000300 sec
D1 1.0000000 sec
D11 0.0300000 sec
D12 0.0002000 sec
D13 0.0000400 sec
D16 0.0002000 sec
SFO1 500.1323623 MHz

===== CHANNEL f1 =====
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NUC1 1H
P0 13.35 usec
P1 13.35 usec
P17 2500.00 usec
PL1 16.00000000 W
PL10 3.16840005 W

===== GRADIENT CHANNEL =====
GPRAM[1] SMSQ10.100
GPS1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 500.1324 MHz
FIDRES 33.614608 Hz
SW 8.404 ppm
FWDGGE QF

F2 - Processing parameters
SI 1024
SF 500.1305132 MHz
WCM QFIME
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1305132 MHz
WCM QFIME
SSB 0
LB 0 Hz
GB 0

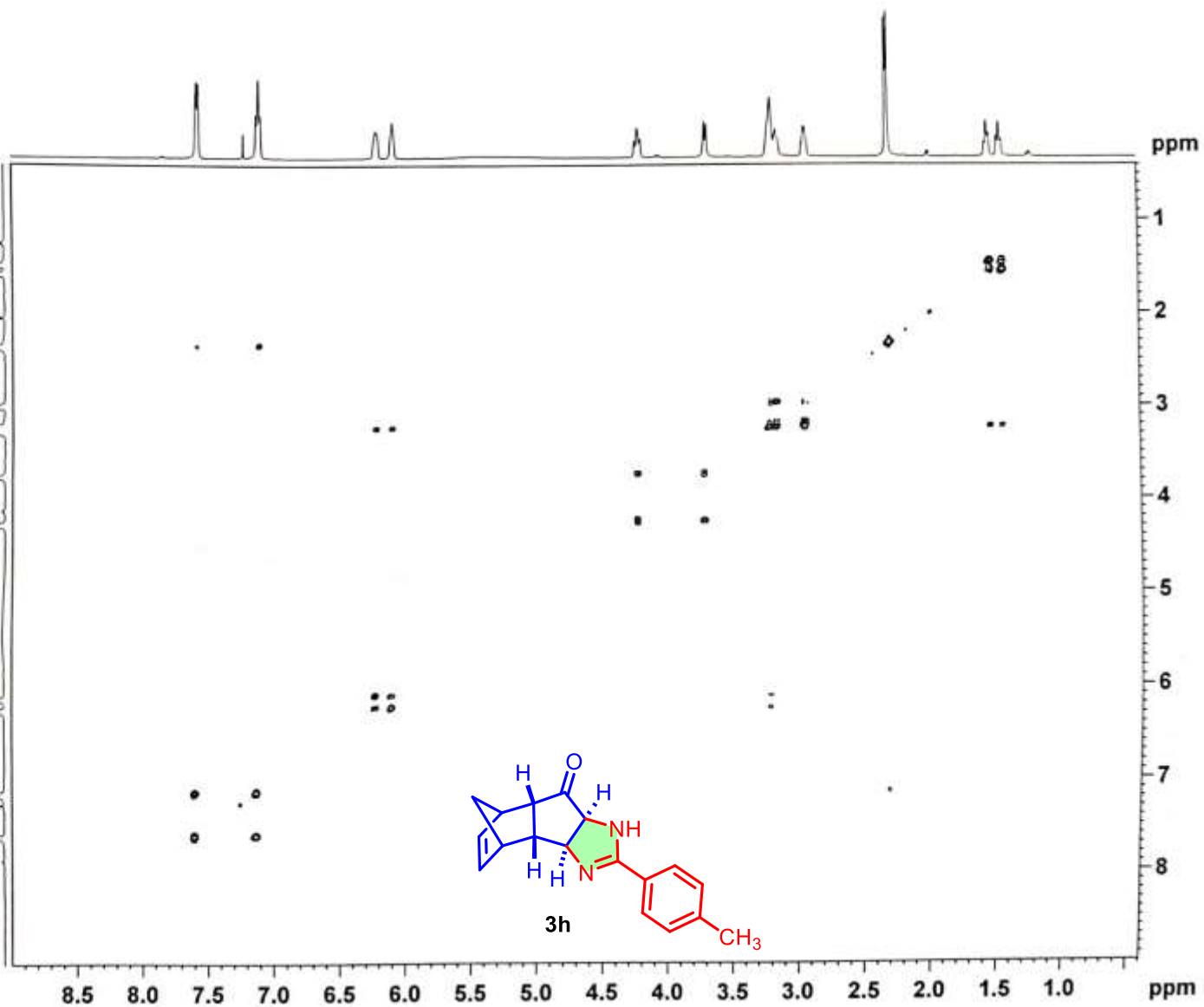


Figure S18. ¹H-¹H COSY NMR of compound 3h

```

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PROCNO 1
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PULPROG zgpg30
TD 32768
SOLVENT H2O
AQ 0.10000000
RG 655
DD 0
FIDRES 0.32000000
AQ 0.10000000
RG 655
DD 0
SFO 500.13622 MHz
NUC1 13C
NUC2 1H
PC 12.00
PF 24.70
PT 1000.00
PL1 0.00000000
===== CHANNEL f1 =====
SFO 500.13622 MHz
NUC1 13C
CPDPRG2 h1_gwagp_3g_2
P1 0.00
P14 500.00
P18 2000.00
P43 1500.00
PLND 0
PLRG 10, 0.00000000
PLM2 1.00000000
SFOA01 Csp40, 4.3, 20.1
SFOA02 0.300
SFOA03 0.00
SFOA04 12.00000000
SFOA05 Csp3, 0.0, 0.500
SFOA06 0.00
SFOA07 10.00000000
SFOA08 Csp3, 1.5, 20.2
SFOA09 0.300
SFOA10 5.00000000
SFOA11 Csp3, 1.5, 20.2
SFOA12 0.500
SFOA13 0.00
SFOA14 3.00000000
===== GRADIENT CHANNEL =====
SFOG01 0.00
SFOG02 0.00
SFOG03 0.00
SFOG04 0.00
SFOG05 0.00
SFOG06 0.00
SFOG07 0.00
SFOG08 0.00
SFOG09 0.00
SFOG10 0.00
SFOG11 0.00
SFOG12 0.00
SFOG13 0.00
SFOG14 0.00
SFOG15 0.00
F1 - Acquisition parameters
TD 32768
SFO 500.13622 MHz
FIDRES 0.32000000
AQ 0.10000000
RG 655
DD 0
SFO 500.13622 MHz
NUC1 13C
NUC2 1H
PC 12.00
PF 24.70
PT 1000.00
PL1 0.00000000
===== CHANNEL f2 =====
SFO 125.76140 MHz
NUC1 13C
CPDPRG2 h1_gwagp_3g_2
P1 0.00
P14 500.00
P18 2000.00
P43 1500.00
PLND 0
PLRG 10, 0.00000000
PLM2 1.00000000
SFOA01 Csp40, 4.3, 20.1
SFOA02 0.300
SFOA03 0.00
SFOA04 12.00000000
SFOA05 Csp3, 0.0, 0.500
SFOA06 0.00
SFOA07 10.00000000
SFOA08 Csp3, 1.5, 20.2
SFOA09 0.300
SFOA10 5.00000000
SFOA11 Csp3, 1.5, 20.2
SFOA12 0.500
SFOA13 0.00
SFOA14 3.00000000
===== GRADIENT CHANNEL =====
SFOG01 0.00
SFOG02 0.00
SFOG03 0.00
SFOG04 0.00
SFOG05 0.00
SFOG06 0.00
SFOG07 0.00
SFOG08 0.00
SFOG09 0.00
SFOG10 0.00
SFOG11 0.00
SFOG12 0.00
SFOG13 0.00
SFOG14 0.00
SFOG15 0.00
F2 - Processing parameters
SI 32768
SF 500.13622 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.00
F3 - Processing parameters
SI 32768
SF 125.76140 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.00

```

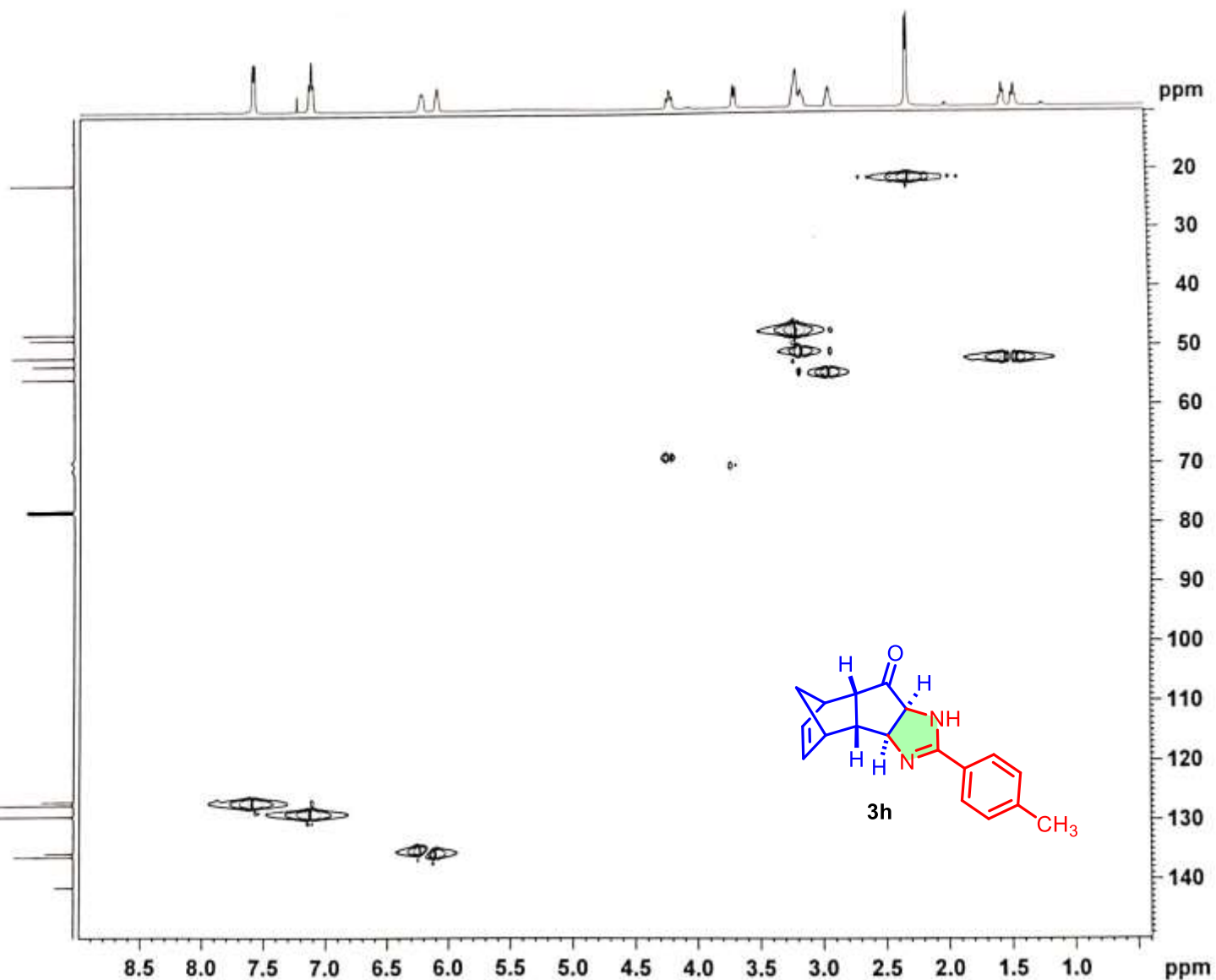


Figure S19. ¹H-¹³C HSQC NMR of compound 3h

INN-SOHAN-II-189C-1H

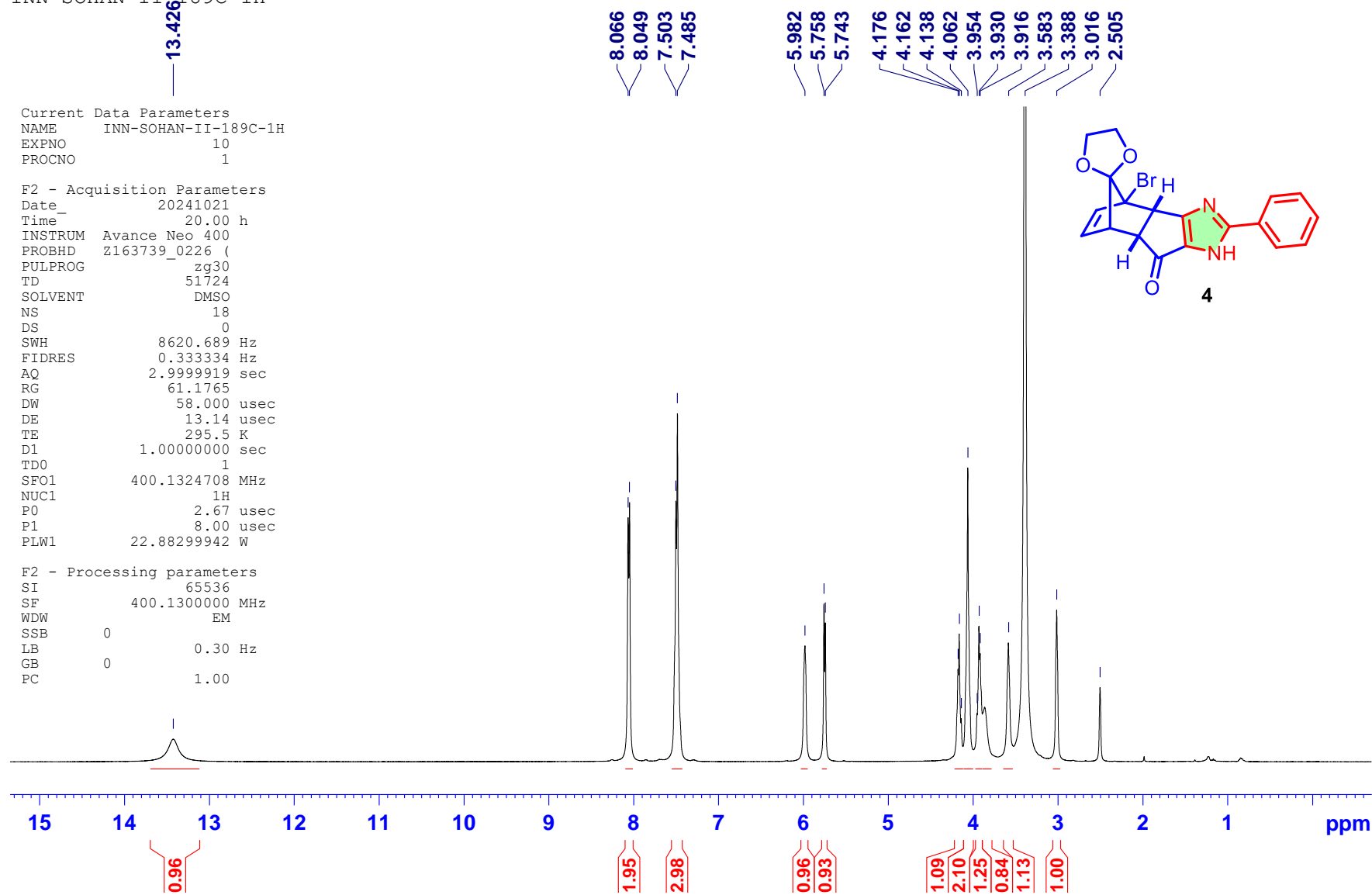


Figure S20. ¹H NMR of compound 4

INN-TGL-04-56-APT

Current Data Parameters
NAME INN-TGL-04-56-APT
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20260130
Time_ 9.25 h
INSTRUM Avance Neo 400
PROBHD Z163739_0226 (
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 14284
DS 0
SWH 27777.778 Hz
FIDRES 0.847710 Hz
AQ 1.1796480 sec
RG 101
DW 18.000 usec
DE 6.50 usec
TE 296.6 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
D20 0.00689655 sec
TD0 1
SFO1 100.6242384 MHz
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 97.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 25.07999992 W
PLW12 0.19815999 W

F2 - Processing parameters
SI 32768
SF 100.6127906 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

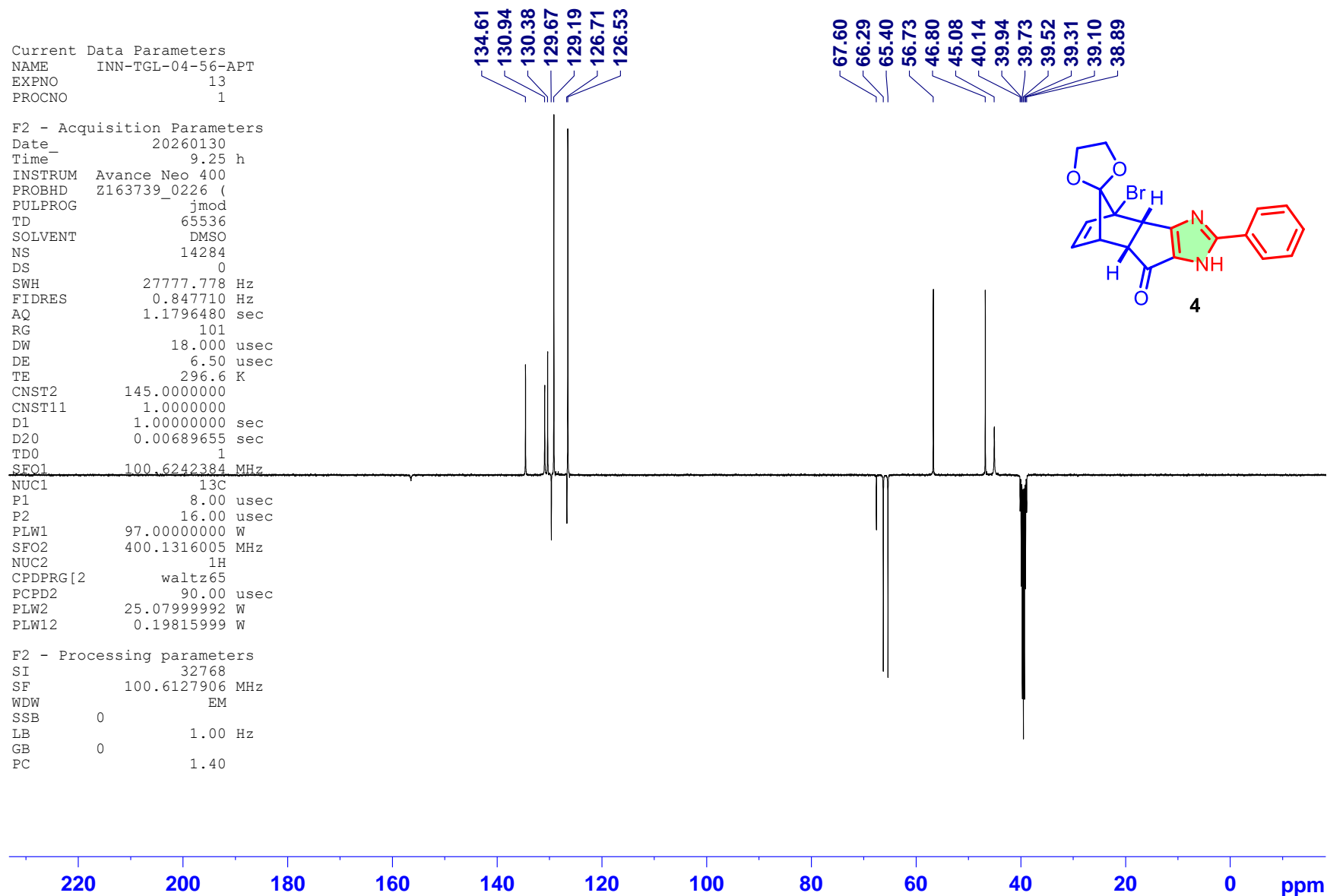


Figure S22. ¹³C-APT NMR of compound 4

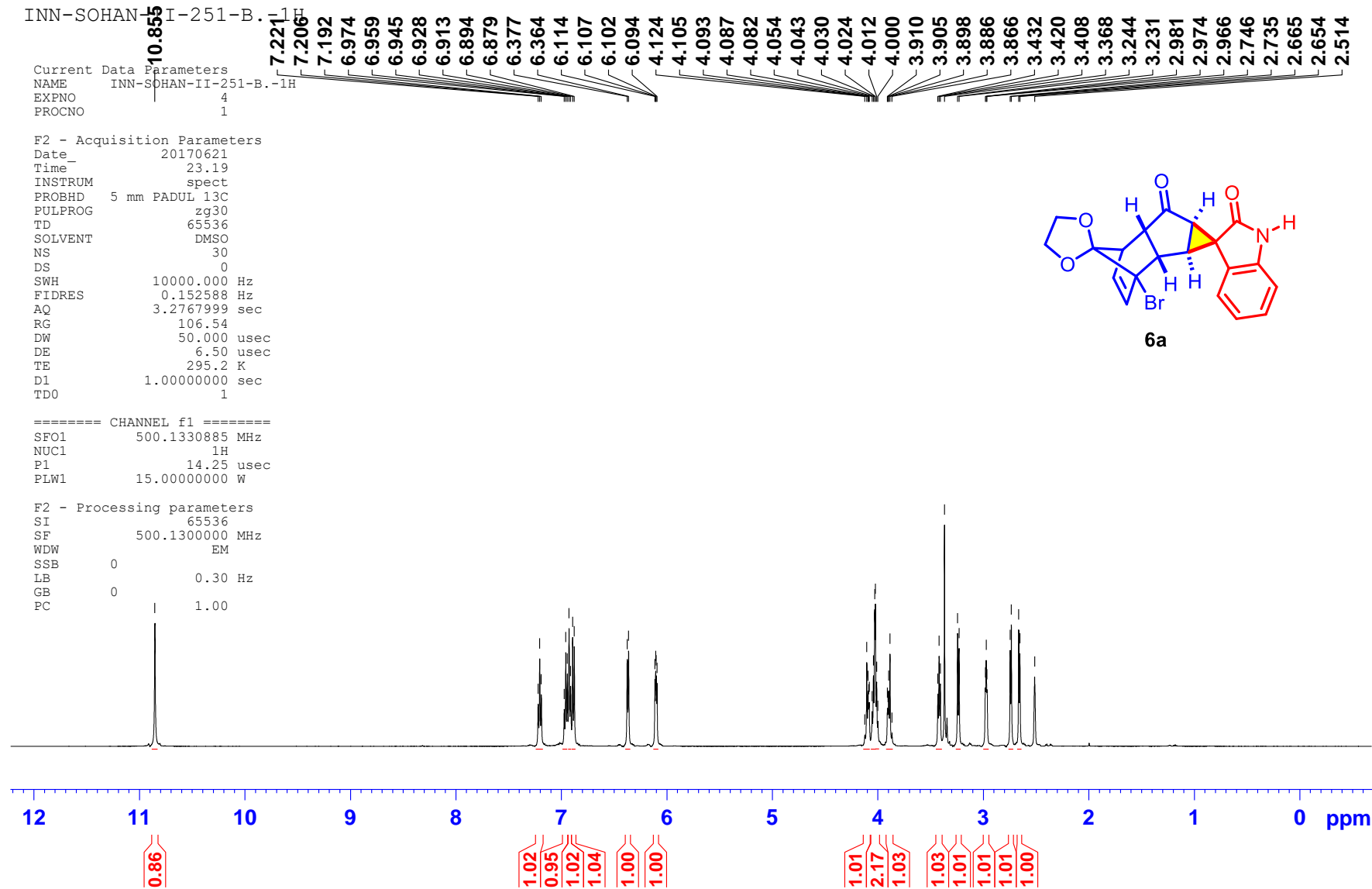


Figure S23. ¹H NMR of compound **6a**

INN-SOHAN-II-251-B-13C

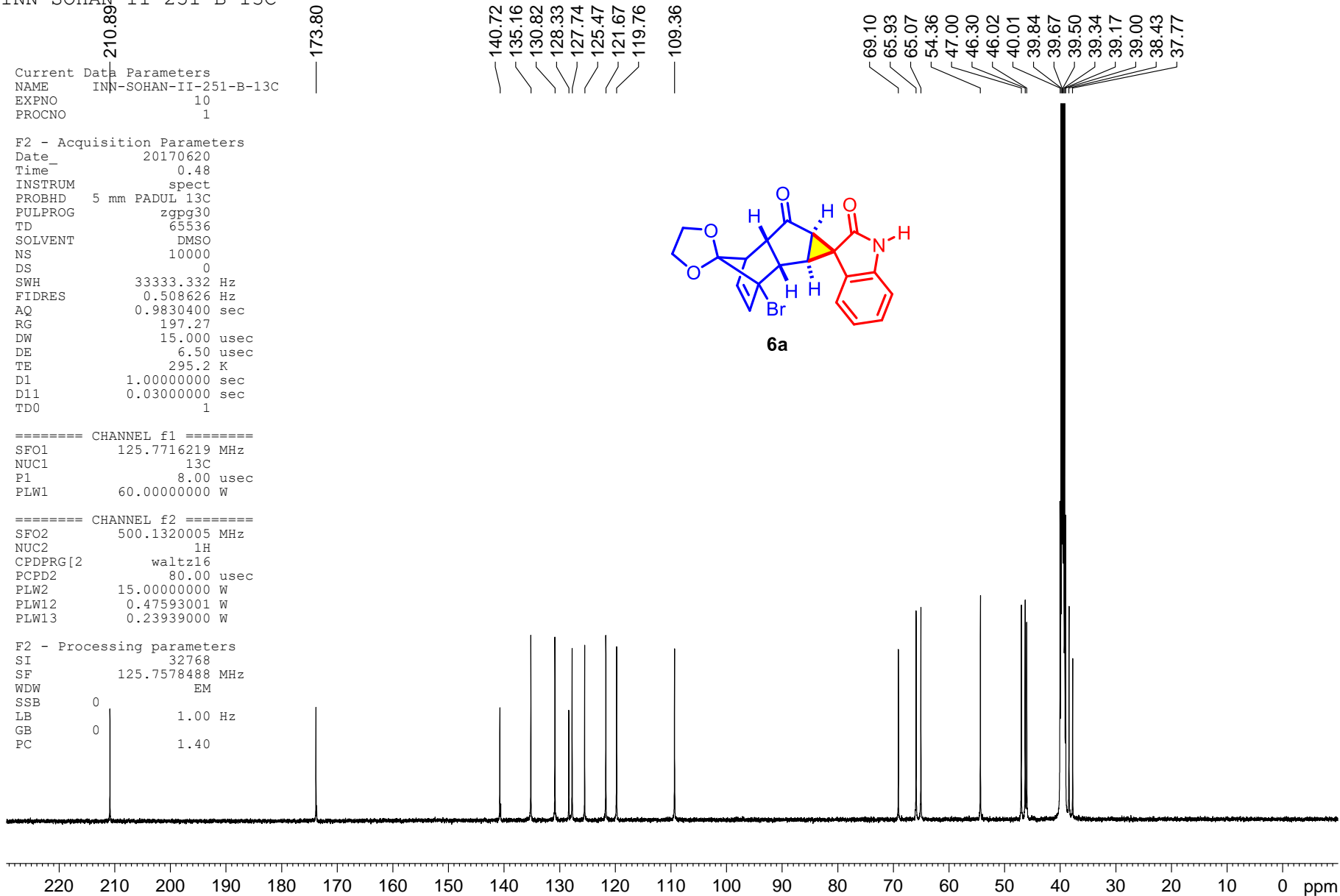


Figure S24. ¹³C NMR of compound 6a

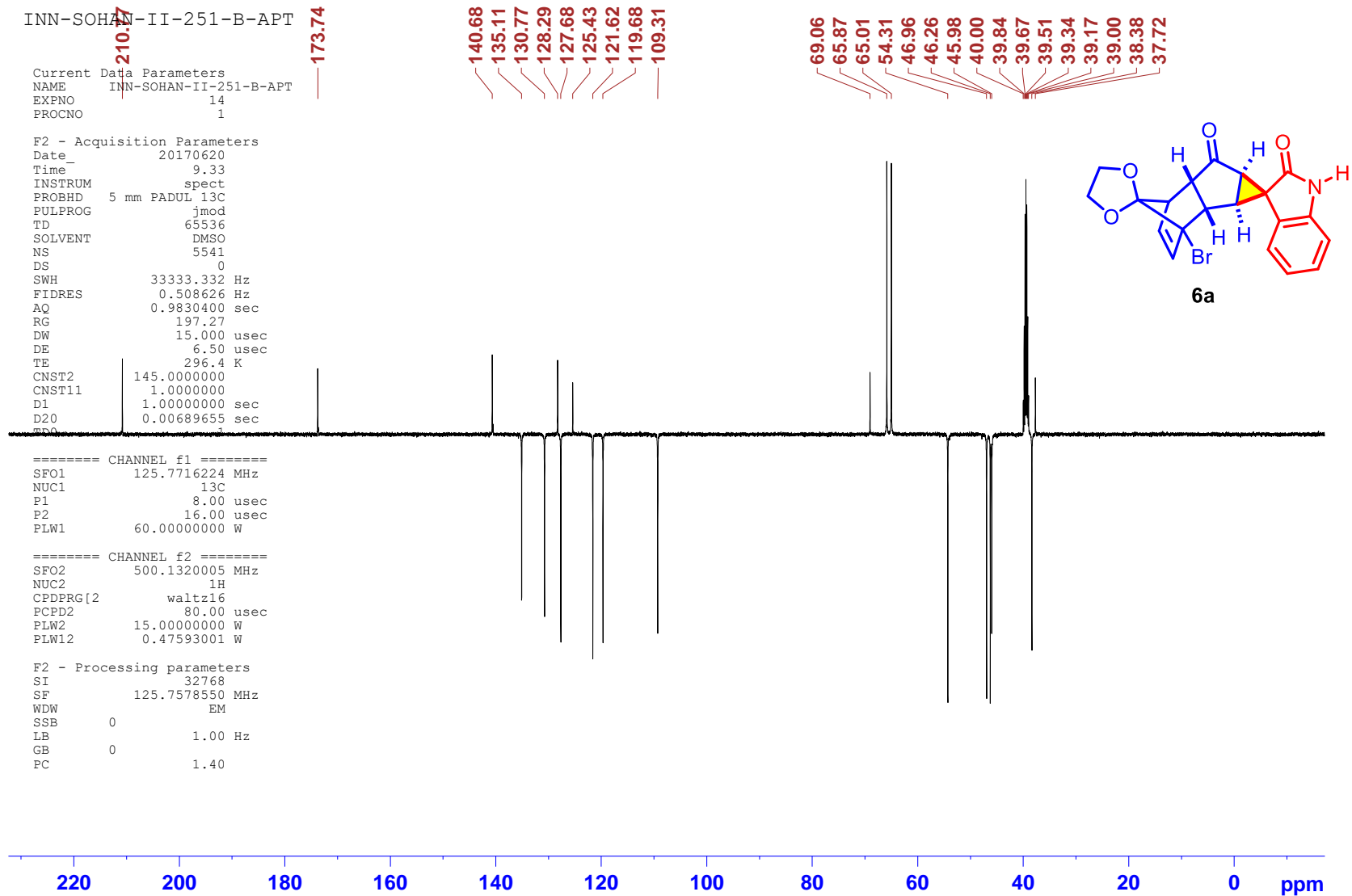
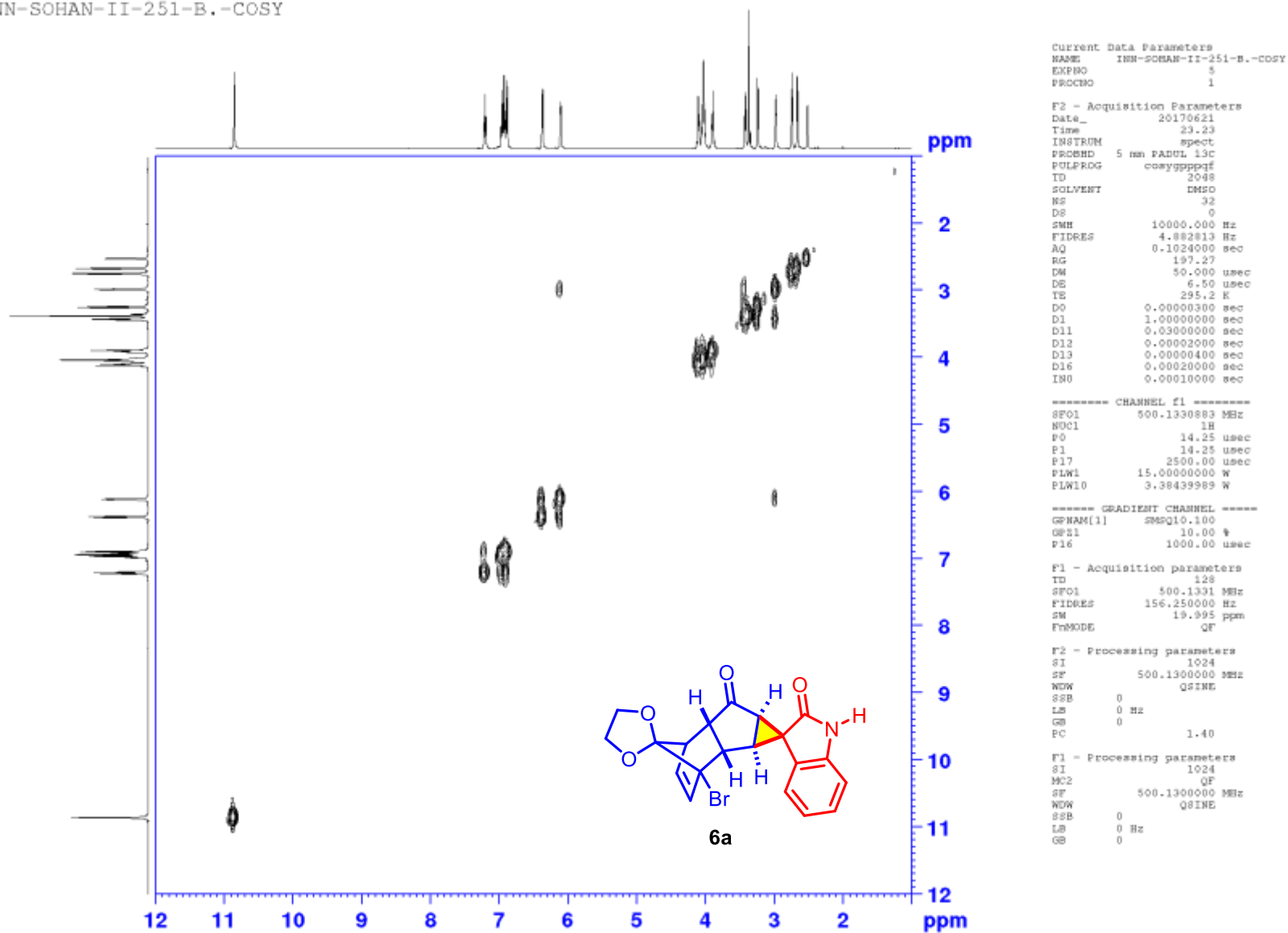
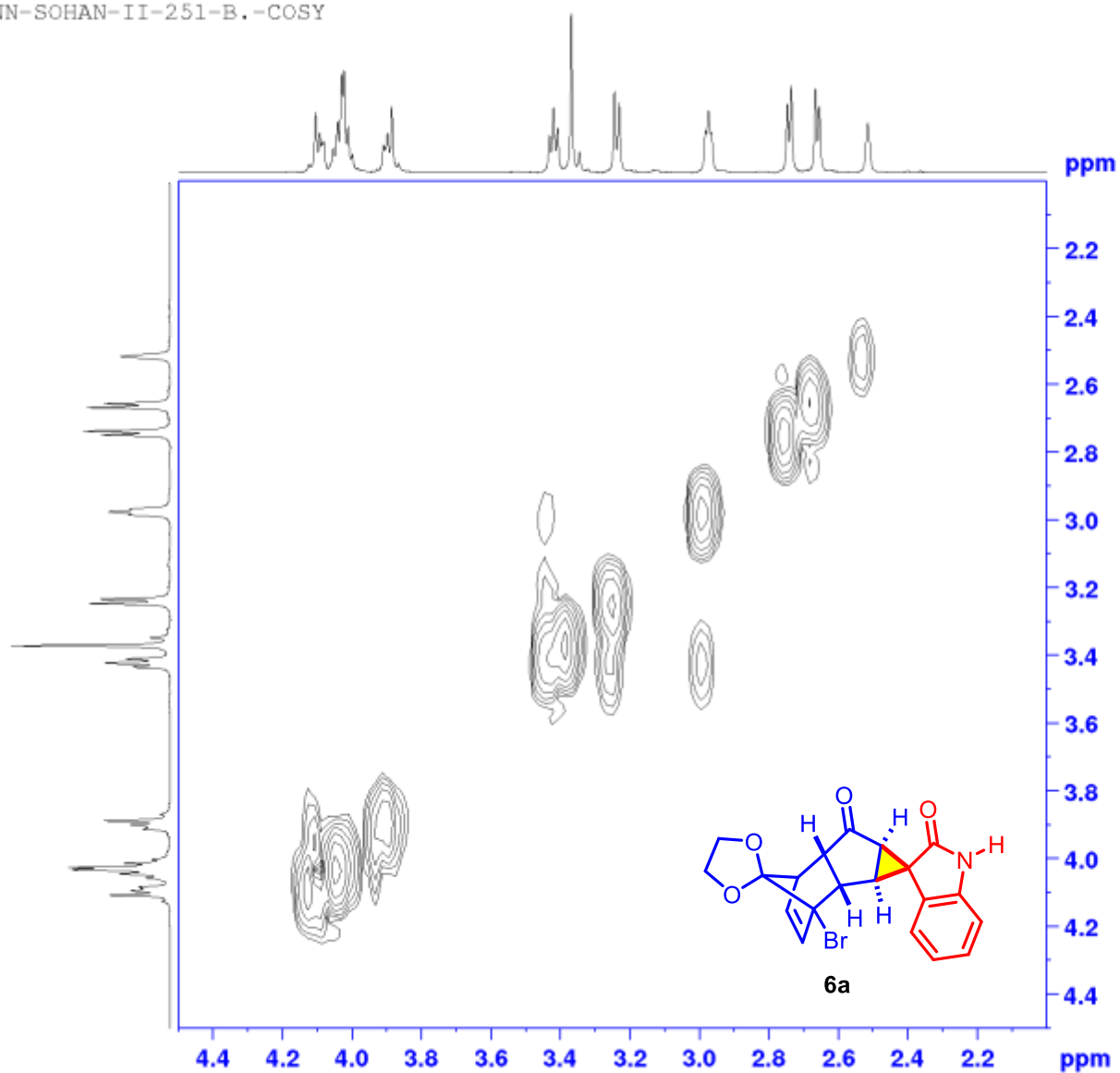


Figure S25. ¹³C-APT NMR of compound 6a

Figure S26. ^1H - ^1H COSY NMR of compound 6a

INN-SOHAN-II-251-B.-COSY



Current Data Parameters
 NAME INN-SOHAN-II-251-B.-COSY
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170621
 Time 23.23
 INSTRUM spect
 PROCNO 5 mm PADUL 13C
 PULPROG cosygppppqf
 ID 2048
 SOLVENT DMSO
 NS 32
 DS 0
 SMN 10000.000 Hz
 FIDRES 4.882813 Hz
 AQ 0.1024000 sec
 RG 197.27
 DM 50.000 usec
 DE 6.50 usec
 TE 295.2 K
 DO 0.00000300 sec
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00000000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00010000 sec

----- CHANNEL f1 -----
 SFO1 500.1330883 MHz
 NUCL1 1H
 P0 14.25 usec
 P1 14.25 usec
 P17 2500.00 usec
 PLW1 15.00000000 W
 PLW10 3.38439989 W

----- GRADIENT CHANNEL -----
 GPMAX[1] SMSQ10.100
 GPC1 10.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 500.1331 MHz
 FIDRES 156.250000 Hz
 SW 19.995 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 500.1300000 MHz
 WDW QSINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.1300000 MHz
 WDW QSINE
 SSB 0
 LB 0 Hz
 GB 0

Figure S26a. Expansion of ¹H-¹H COSY NMR of compound 6a

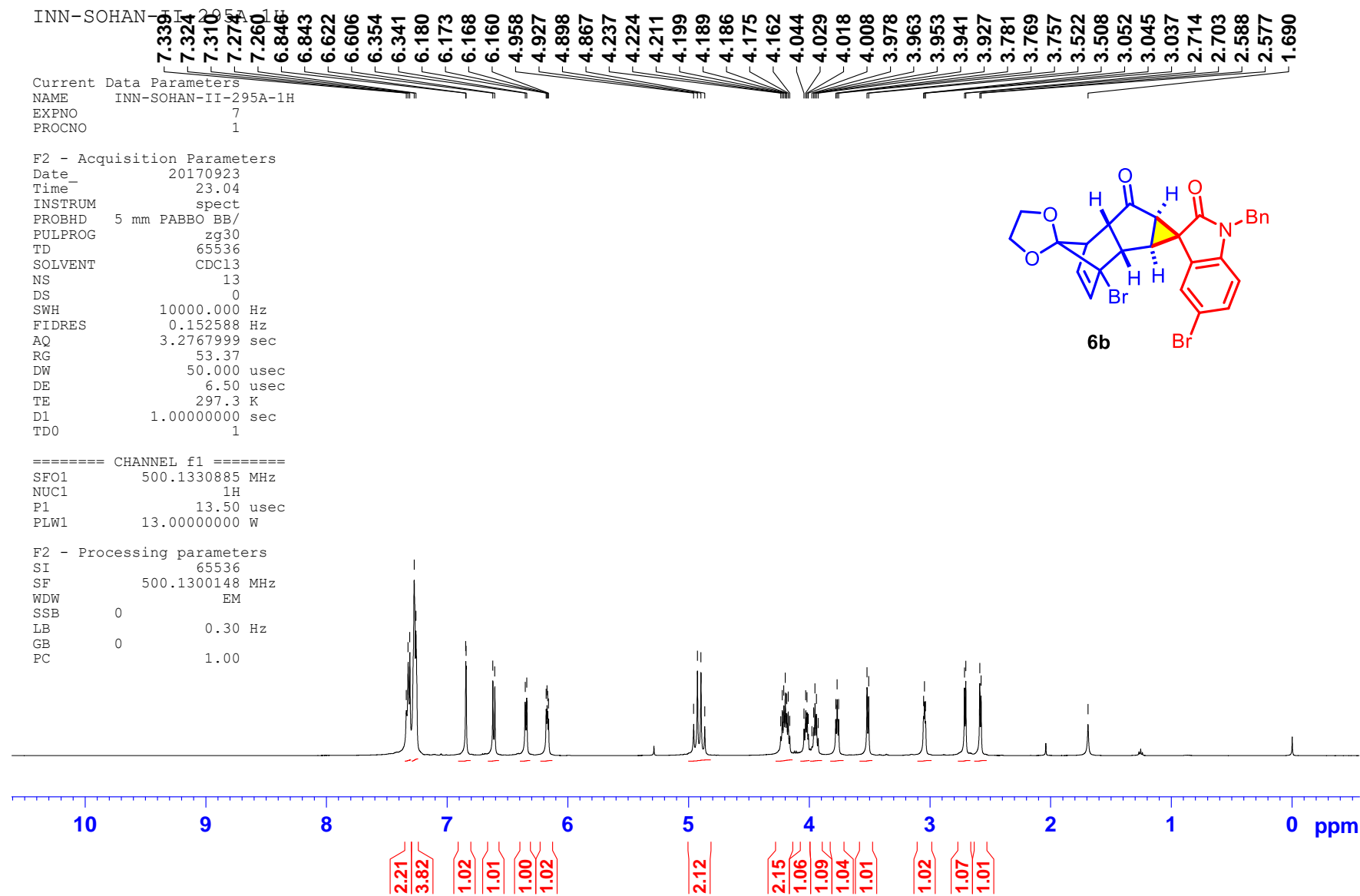


Figure S28. ¹H NMR of compound **6b**

INN-SOHAN-II-295A-13C

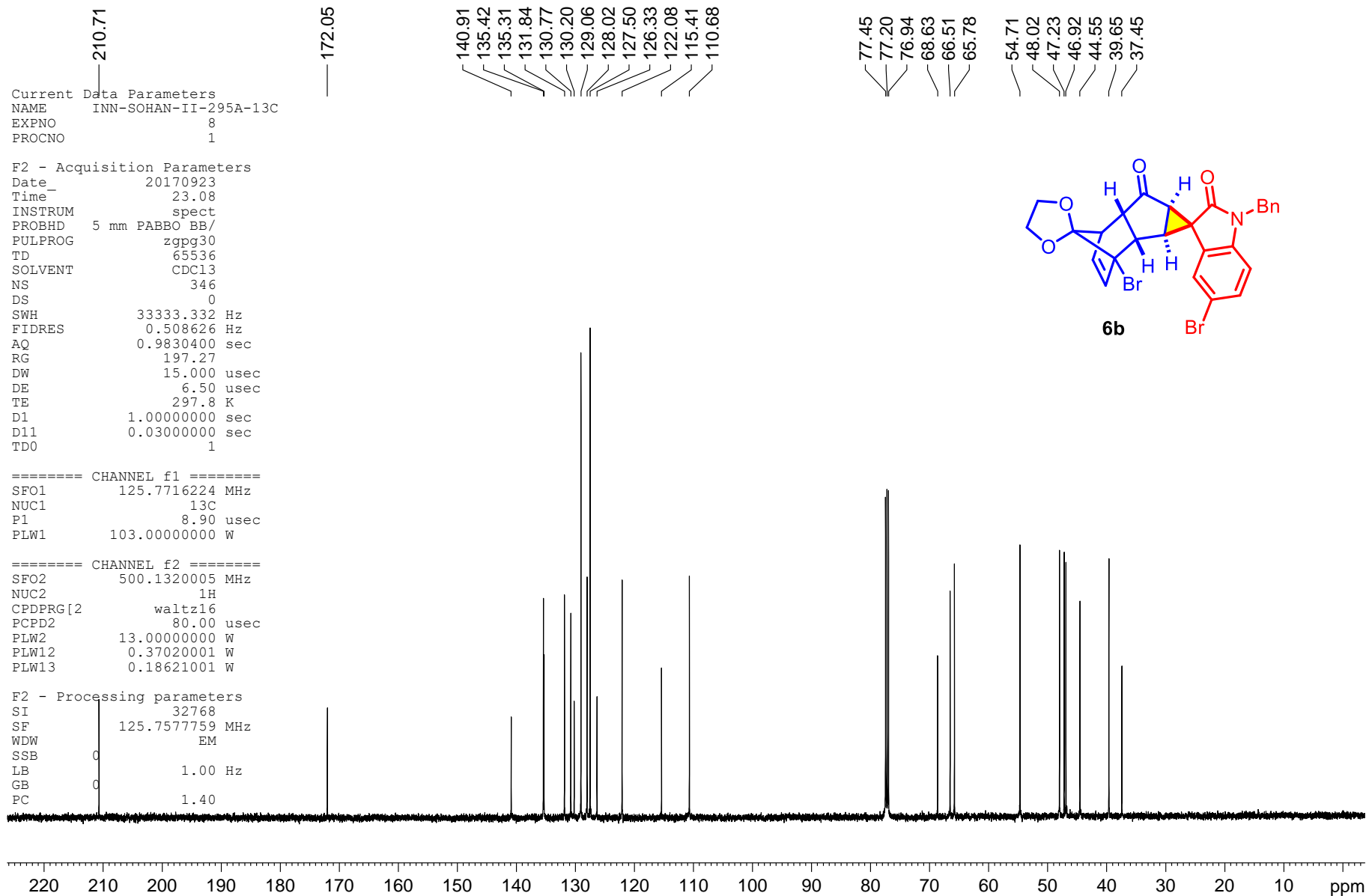


Figure S29. ¹³C NMR of compound **6b**

INN-SOHAN-II-295A-APT

Current Data Parameters
NAME INN-SOHAN-II-295A-APT
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170923
Time_ 23.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG jmod
TD 65536
SOLVENT CDC13
NS 215
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 197.27
DW 15.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
D20 0.00689655 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7716224 MHz
NUC1 13C
P2 17.80 usec
PLW1 103.00000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 13.00000000 W
PLW12 0.37020001 W

F2 - Processing parameters
SI 32768
SF 125.7577758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

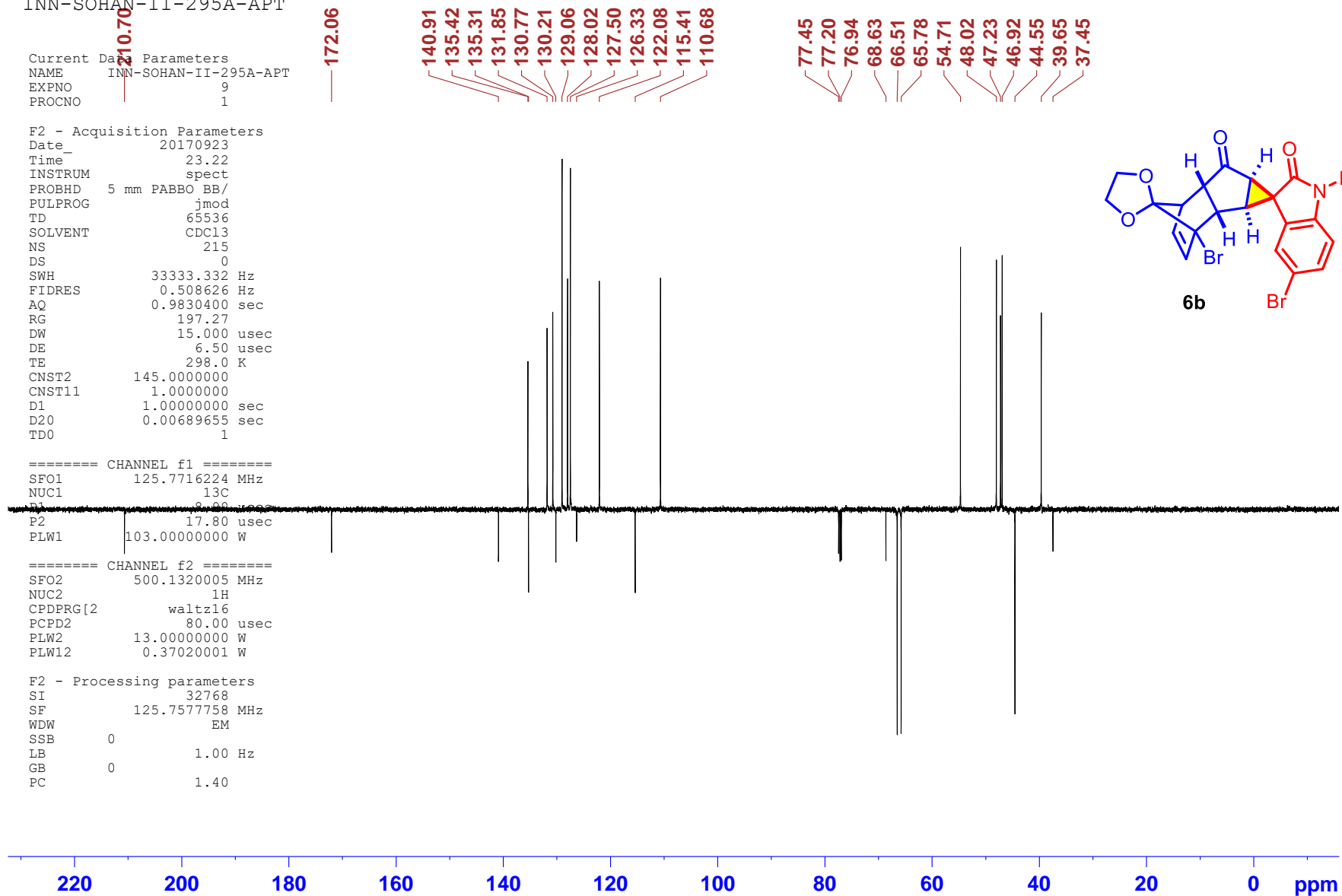


Figure S30. ¹³C-APT NMR of compound 6b

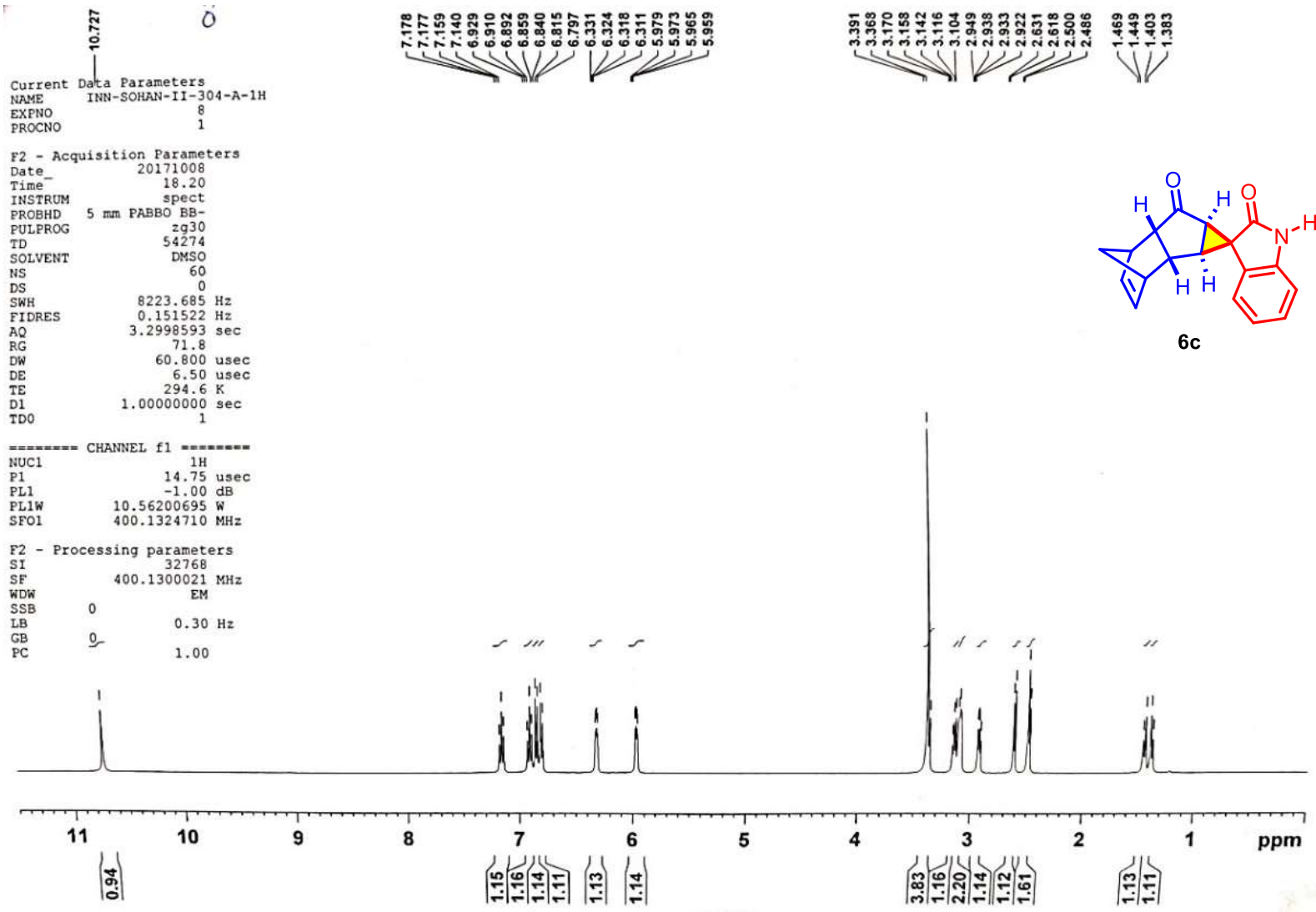


Figure S31. ¹H NMR of compound 6c

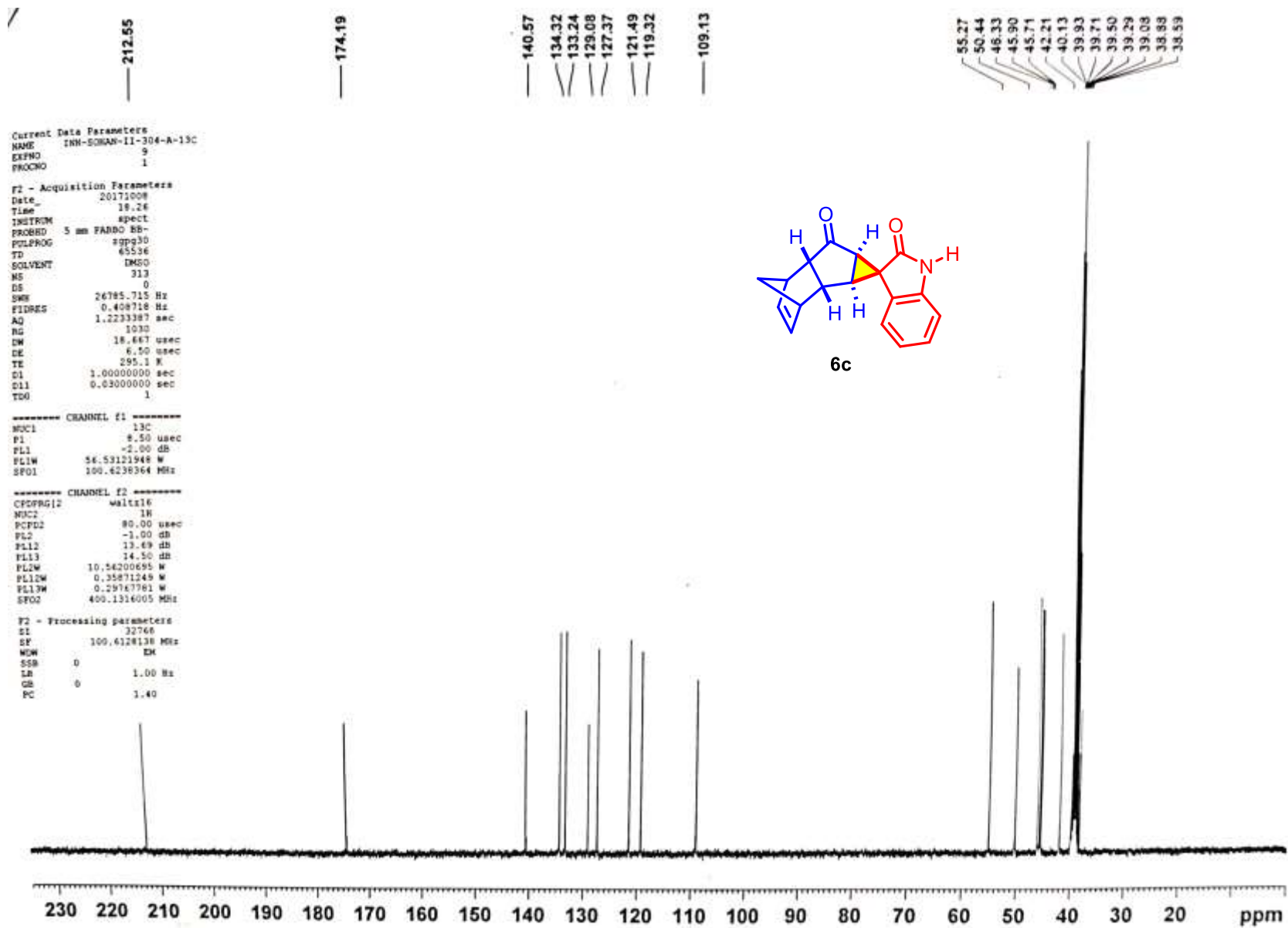


Figure S32. ¹³C NMR of compound 6c

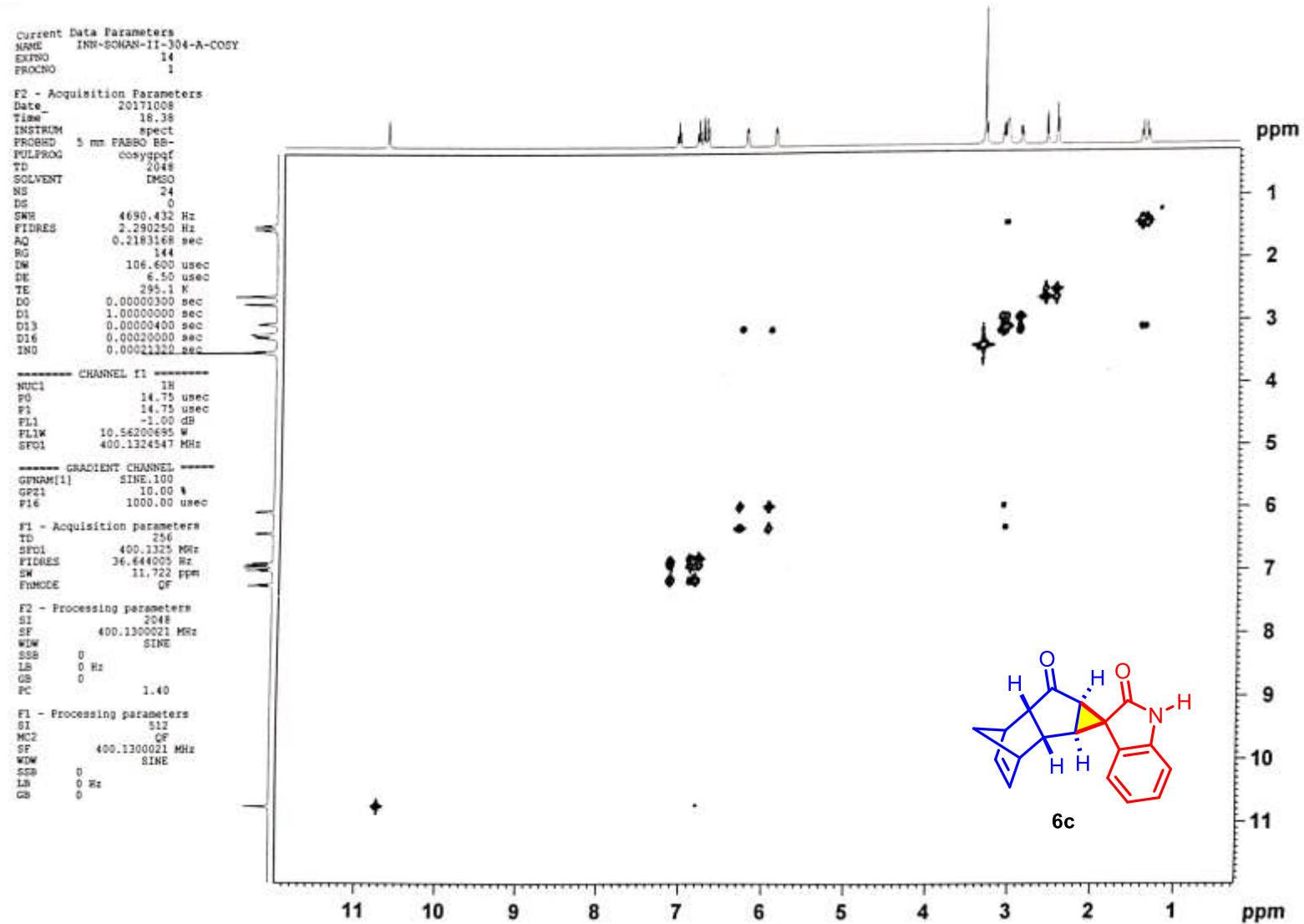


Figure S33. ^1H - ^1H COSY NMR of compound **6c**

```

Current Data Parameters
NAME      IHW-SONAM-II-304-A-HQC
EXPNO    14
PROCNO   1

F2 - Acquisition Parameters
Date_    201708
Time     20.47
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        64
DS        0
SWH       4004.879 Hz
FIDRES   2.248453 Hz
AQ        0.2222763 sec
RG        2050
IN       108.533 usec
DE        6.50 usec
TE        294.4 K
CMT2     145.8050000
D0        0.0000000 sec
D1        1.0000000 sec
D4        0.00172414 sec
D11       0.03000000 sec
D13       0.00000400 sec
D16       0.00020000 sec
IM0       0.00002345 sec
ZGPGPRG  3

===== CHANNEL F1 =====
NUC1      1H
P1        14.75 usec
P2        29.50 usec
P28       0.10 usec
PL1       -1.00 dB
PL18      10.54206495 dB
SFO1      400.1324961 MHz

===== CHANNEL F2 =====
CPDPRG2  gpg3
NUC2      13C
P3        8.50 usec
P4        17.00 usec
PCPD2    70.00 usec
PL2       -2.00 dB
PL12      16.31 dB
PL28      56.53121948 dB
PL18M    0.83423501 dB
SFO2      100.628425 MHz

===== GRADIENT CHANNEL =====
GPMAX[1] 218.100
GPMAX[2] 218.100
GPI1     80.00 %
GPI2     20.20 %
GPI3     1000.00 usec

F1 - Acquisition parameters
TD        65536
SFO1      100.6284 MHz
FIDRES   160.805252 Hz
SW        211.744 ppm
F0MDC5   Echo-Antiecho

F2 - Processing parameters
SI        2048
SF        400.1305021 MHz
WDW       GAUSS
SSB       2
LB        0 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
MC2       echo-antiecho
SF        100.6128138 MHz
WDW       GAUSS
SSB       2
LB        0 Hz
GB        0

```

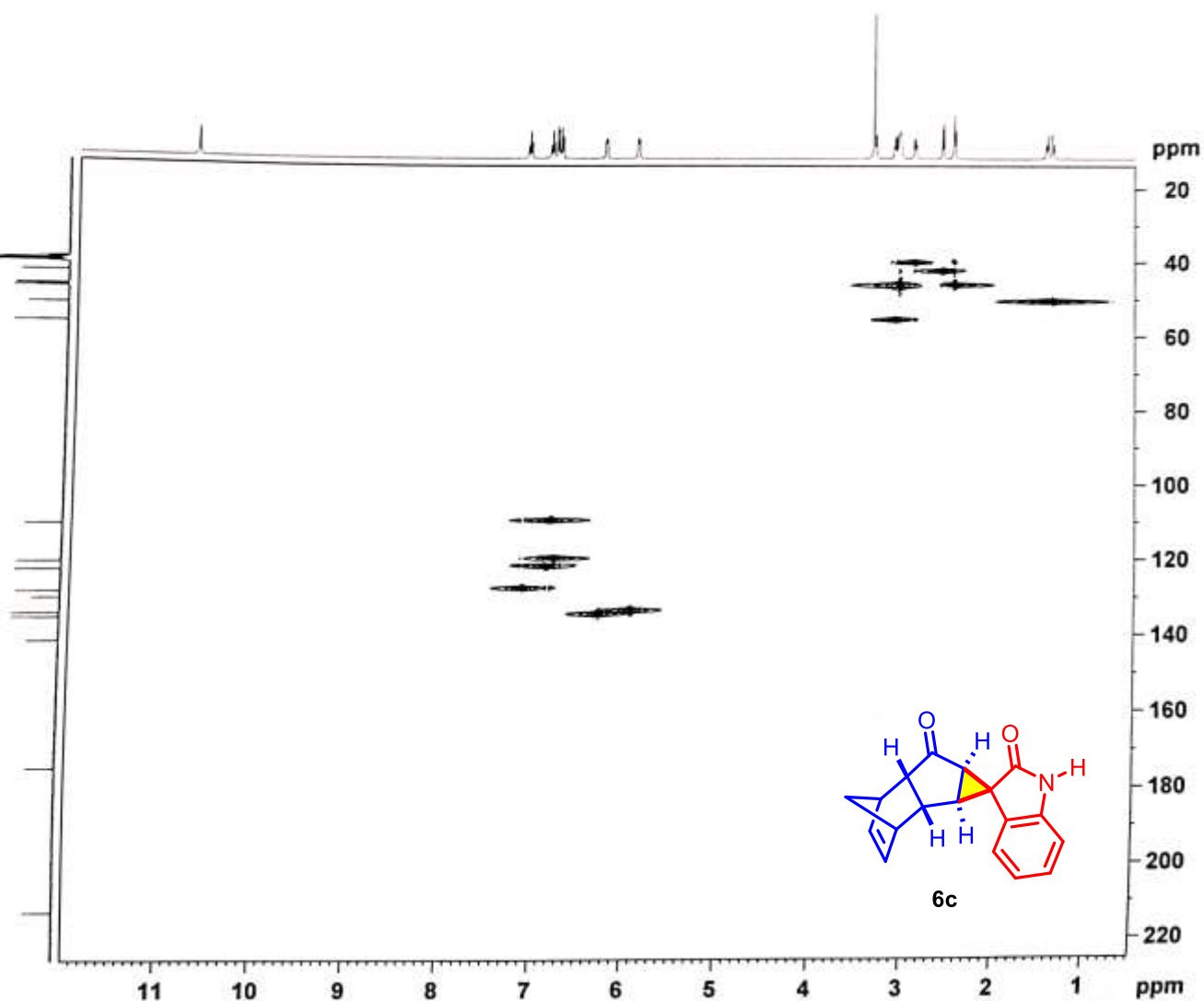


Figure S34. ¹H-¹³C HSQC NMR of compound 6c

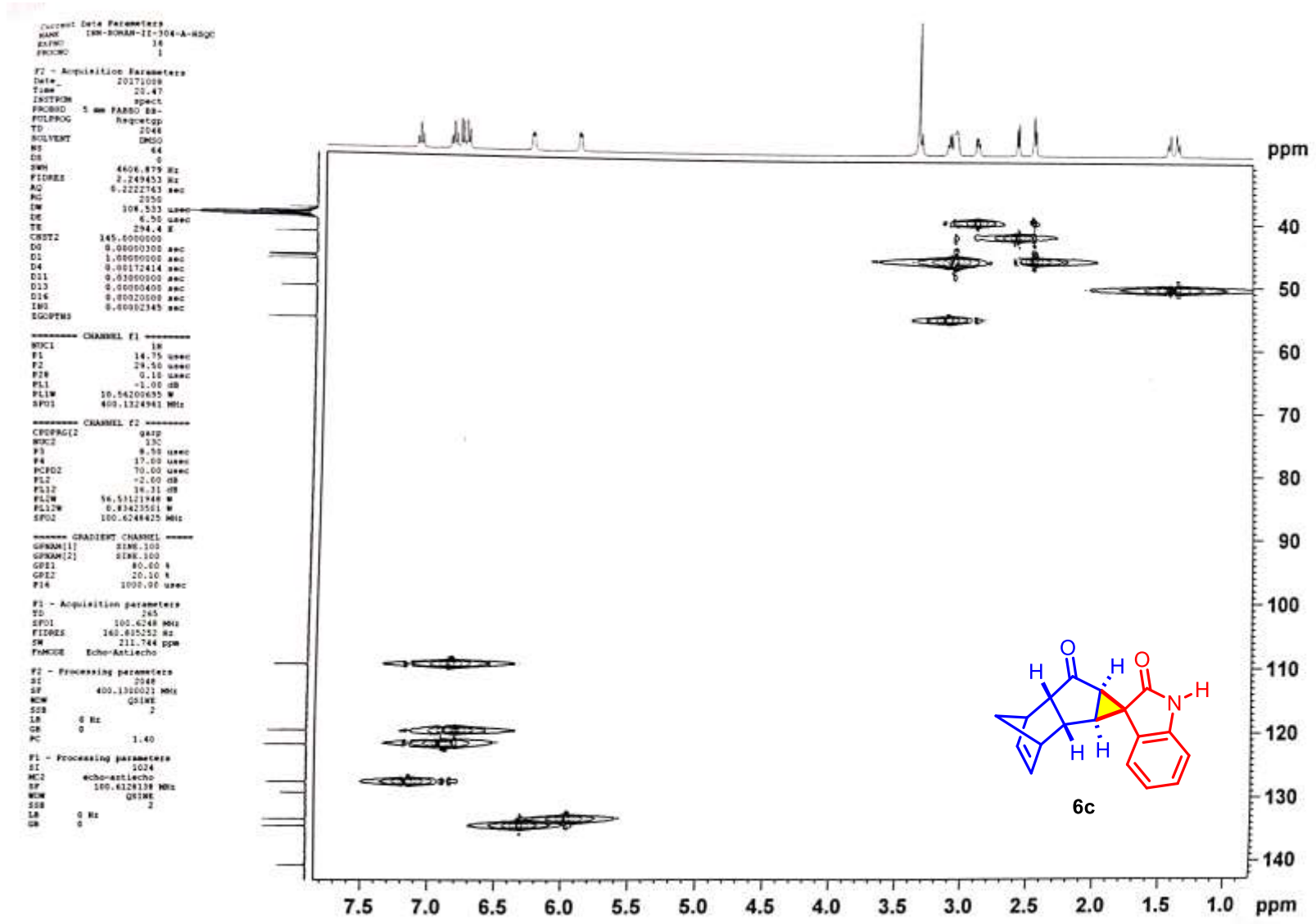


Figure S34a. Expansion of ^1H - ^{13}C HSQC NMR of compound 6c

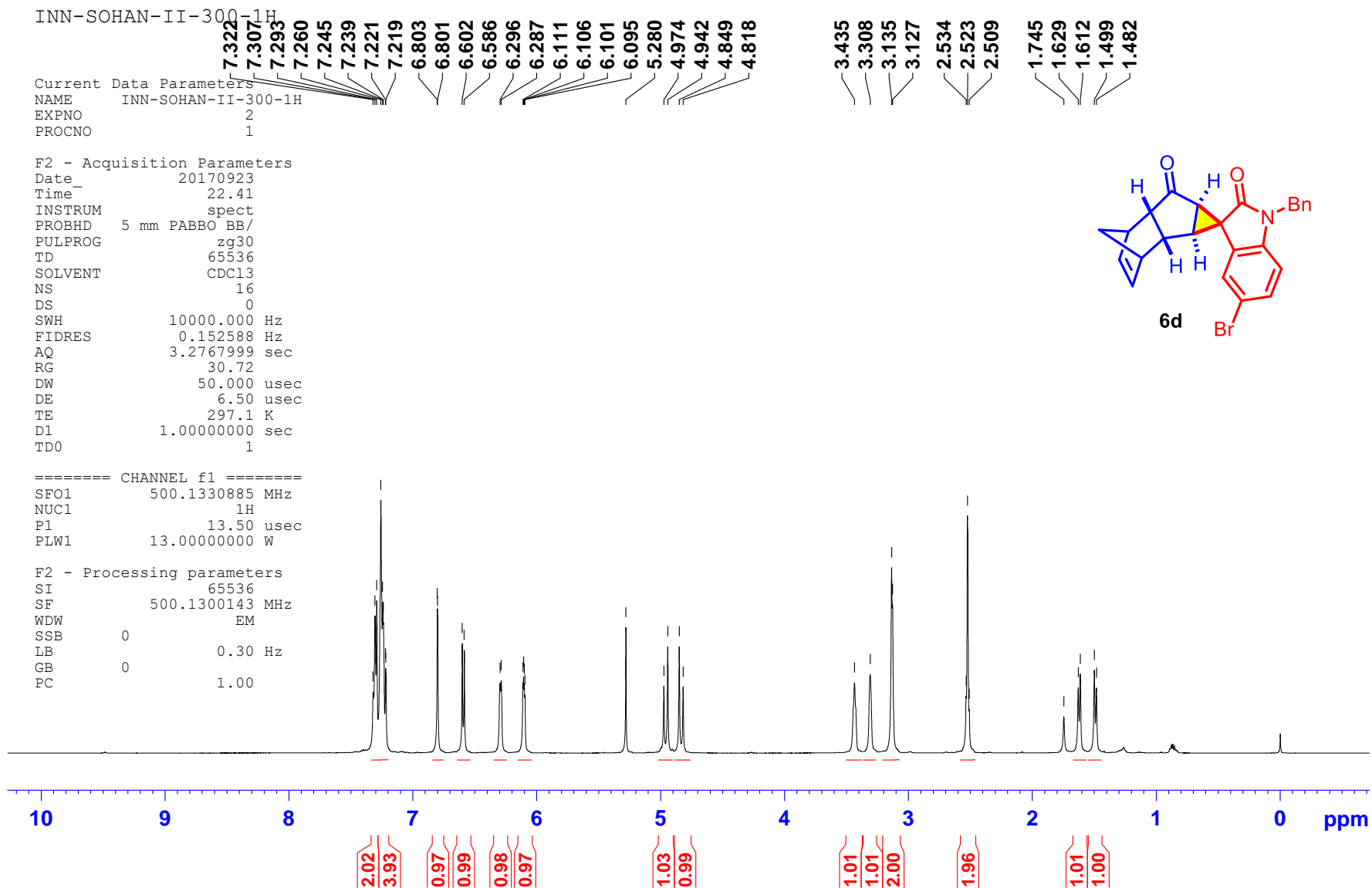


Figure S35. ¹H NMR of compound **6d**

INN-SOHAN-II-300-13C

Current Data Parameters
NAME INN-SOHAN-II-300-13C
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170923
Time_ 22.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 183
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 197.27
DW 15.000 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7716224 MHz
NUC1 13C
P1 8.90 usec
PLW1 103.00000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 13.00000000 W
PLW12 0.37020001 W
PLW13 0.18621001 W

F2 - Processing parameters
SI 32768
SF 125.7577786 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
DC 1.40

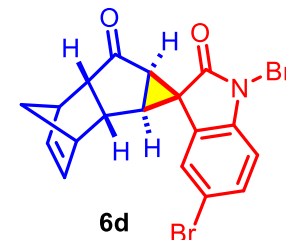
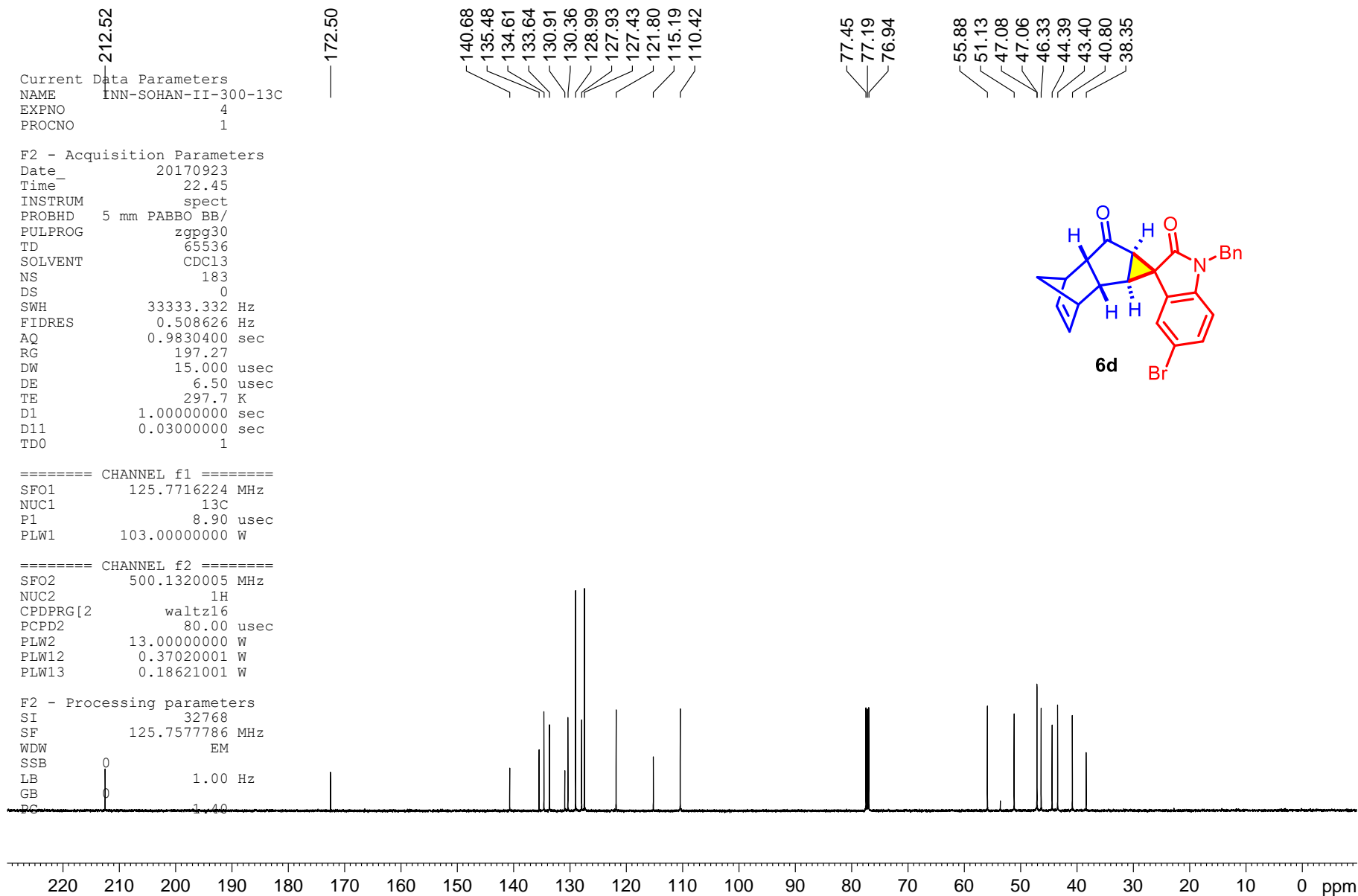


Figure S36. ¹³C NMR of compound **6d**

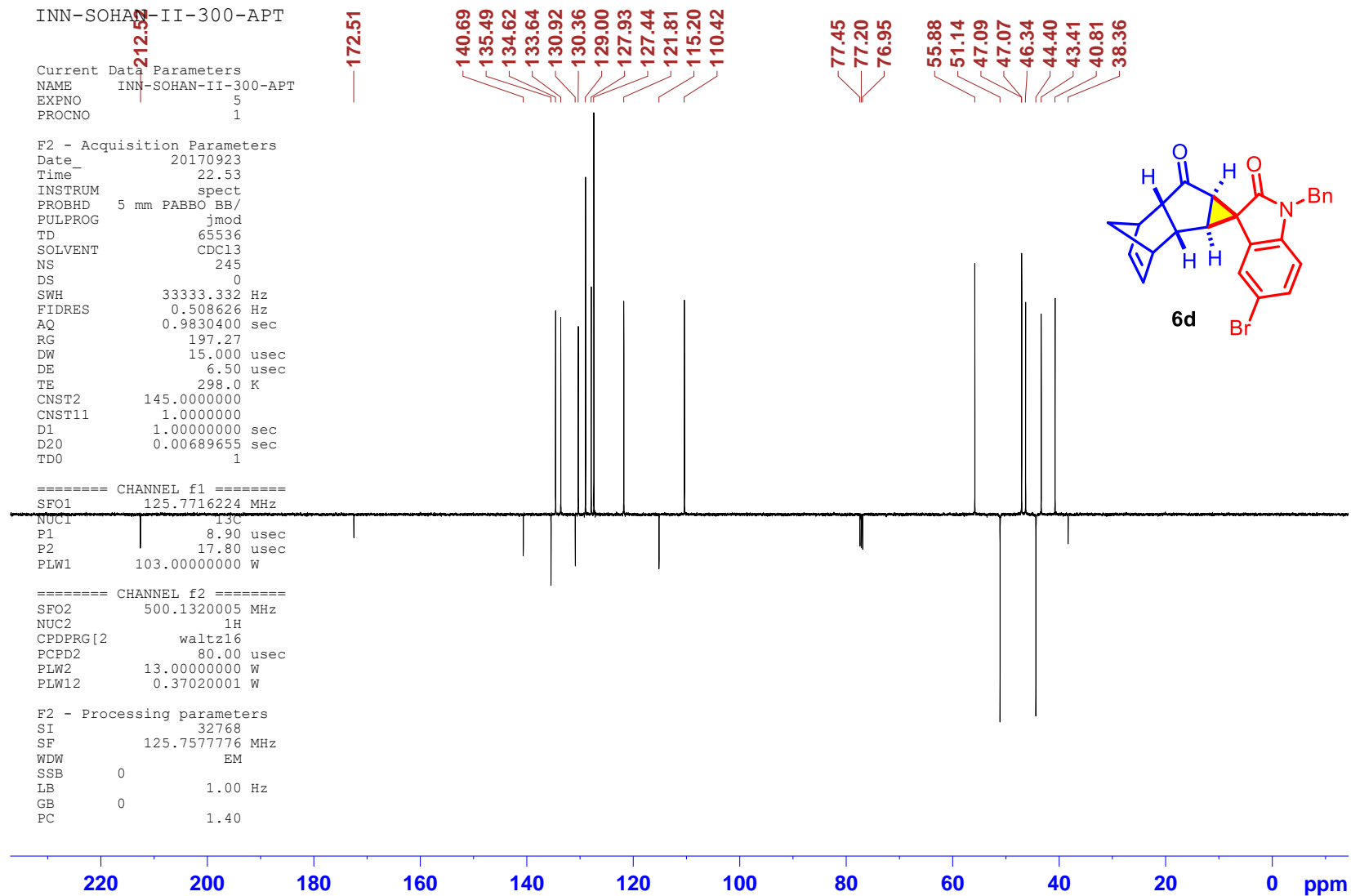


Figure S37. ¹³C-APT NMR of compound 6d

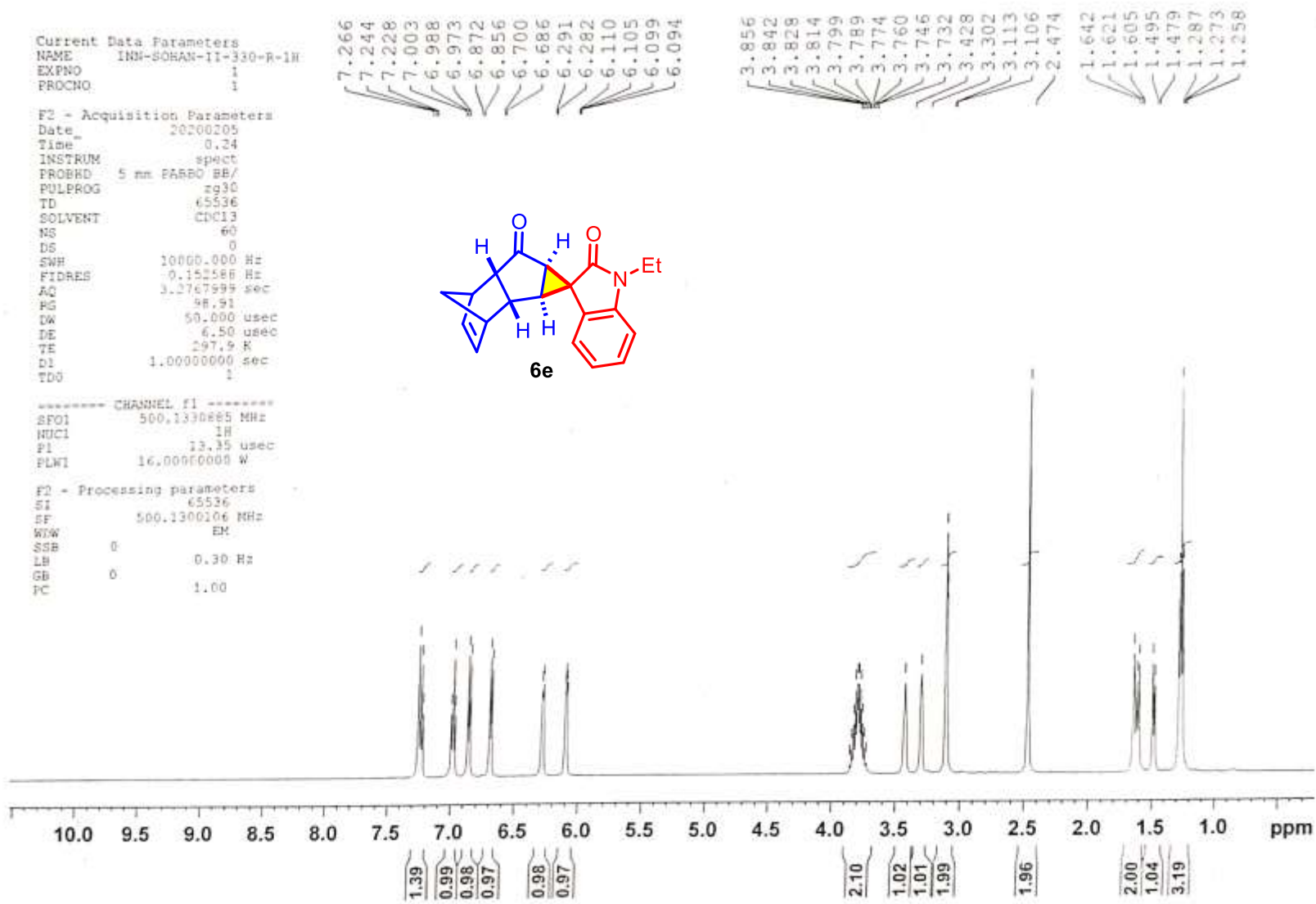


Figure S38. ¹H NMR of compound 6e

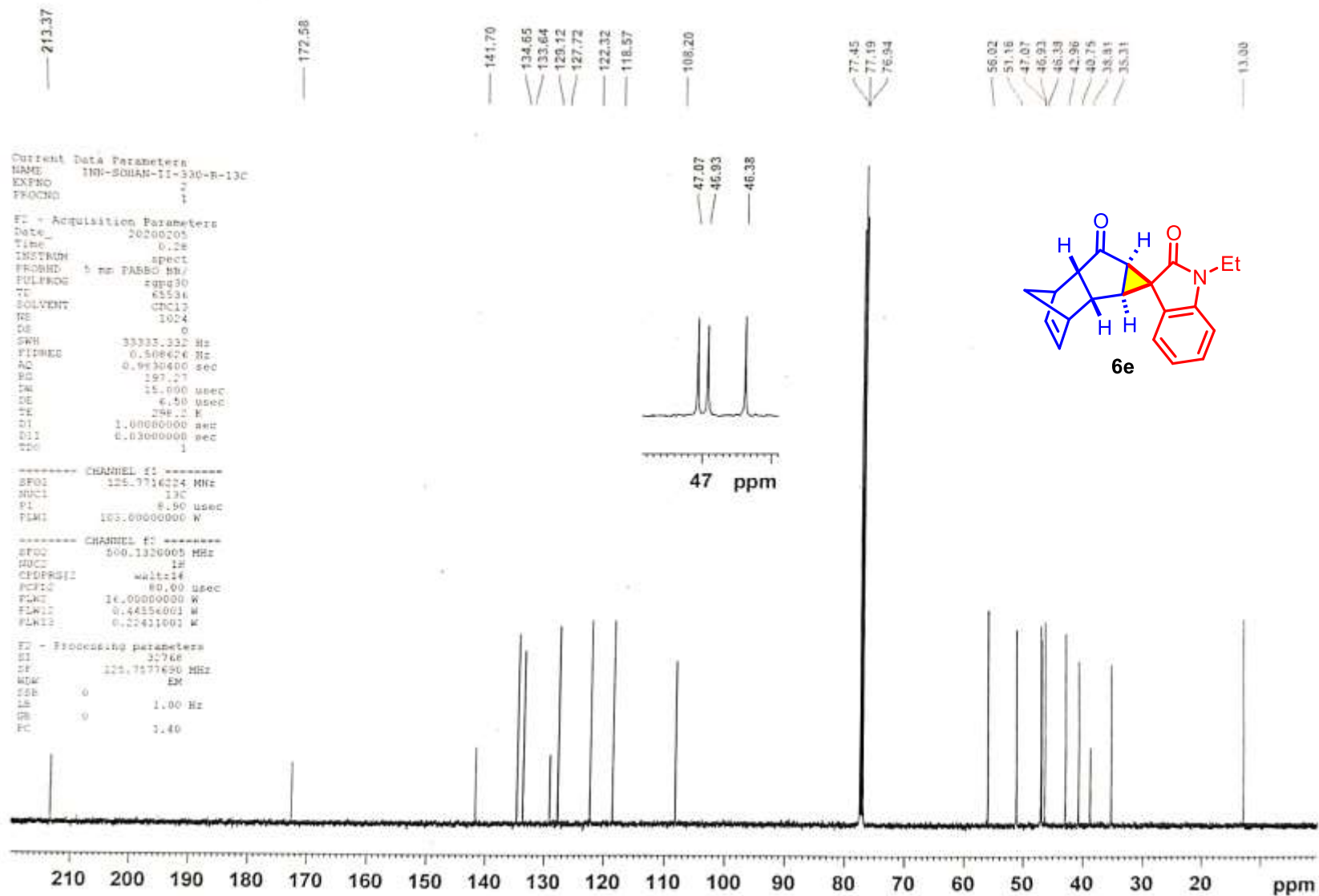


Figure S39. ^{13}C NMR of compound **6e**

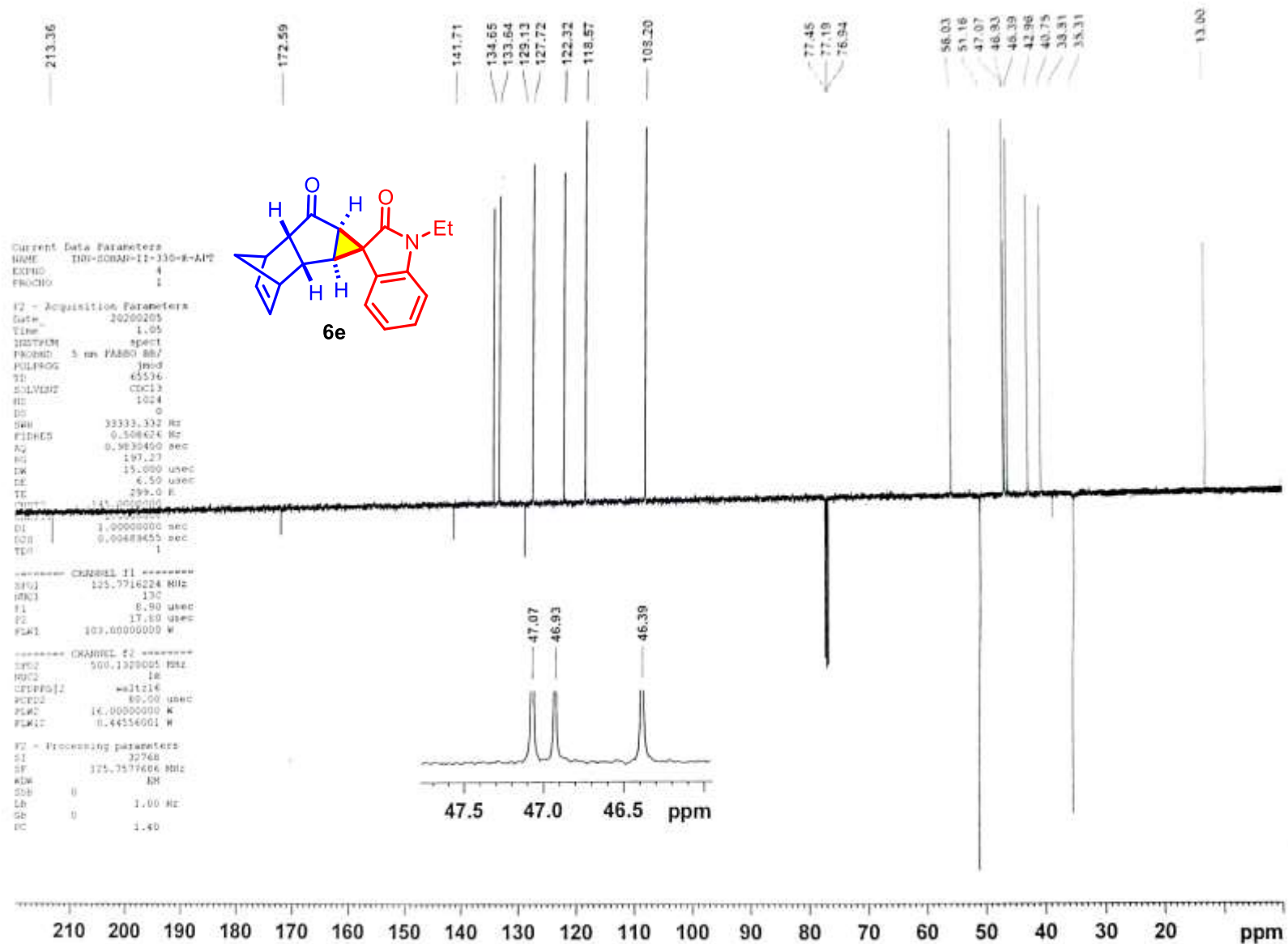


Figure S40. ¹³C-APT NMR of compound **6e**

Current Data Parameters
NAME 11H-COSY-11-330-R-COSY
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20080705
Time 1.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 2048
SOLVENT CDCl3
SI 16
SF 4940.712 Hz
FIDRES 7.412457 Hz
AQ 0.2072574 sec
RG 197.27
DW 101.200 usec
DE 6.50 usec
TE 299.4 K
D0 0.0000000 sec
D1 1.0000000 sec
D11 0.0300000 sec
D12 0.0000000 sec
D13 0.0000400 sec
D14 0.0000000 sec
IND 0.00020249 sec

----- CHANNEL f1 -----

SP01 500.1325484 MHz
NUC1 1H
PC 13.35 usec
PT 13.35 usec
P17 0.0000000 usec
PLM1 14.0000000 W
PLM0 3.14840005 W

----- GRADIENT CHANNEL -----

GRAN11 SMO10.100
GP21 10.00
G14 1070.00 usec

F1 - Acquisition parameters

TD 256
SF01 500.1326 MHz
FIDRES 38.594306 Hz
AQ 9.879 sec
RG0000 0

F2 - Processing parameters

SI 1024
SF 500.1300104 MHz
WDW QOINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
WDW QF
SF 500.1300104 MHz
WDW QOINE
SSB 0
LB 0 Hz
GB 0

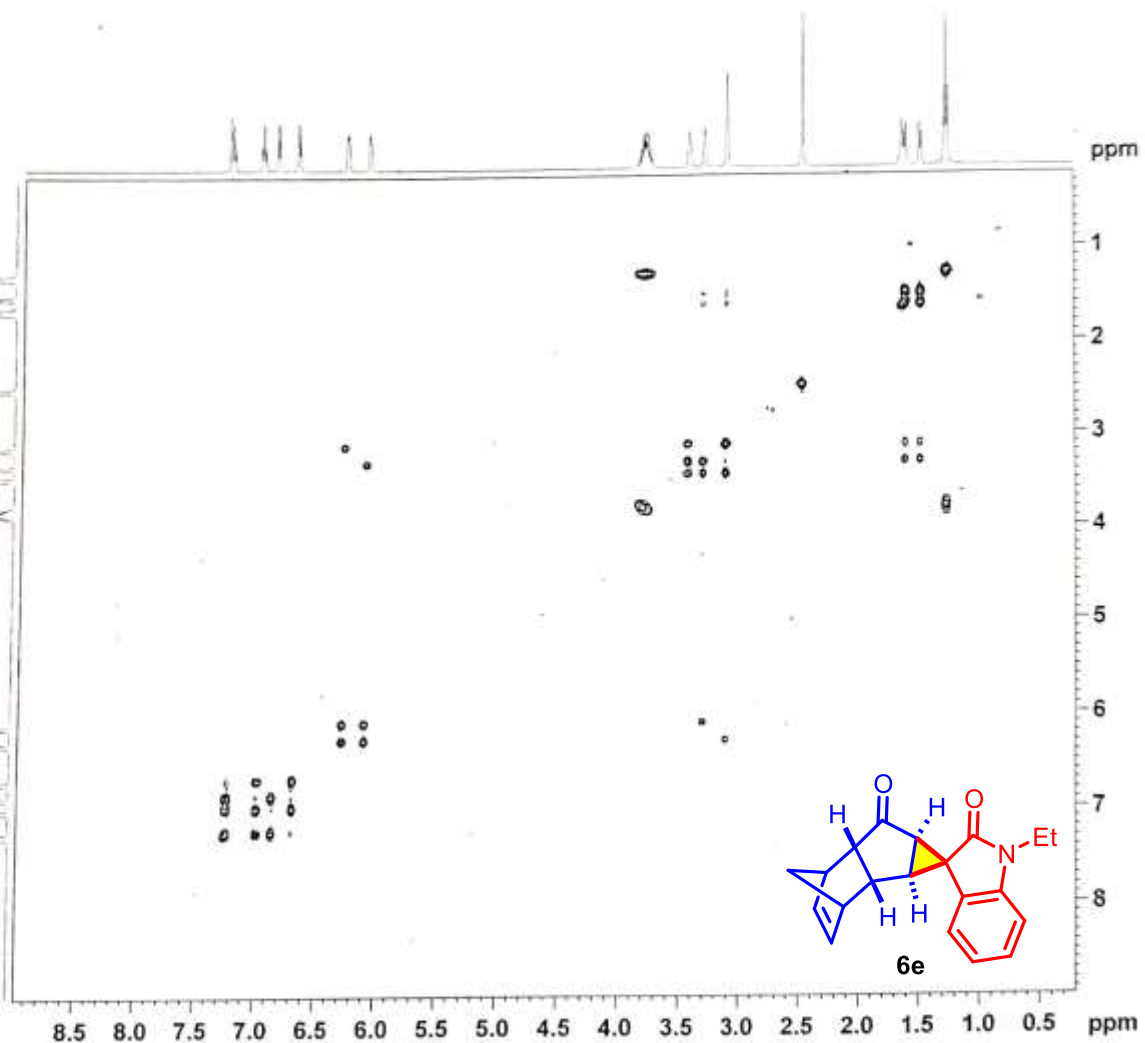


Figure S41. ¹H-¹H COSY NMR of compound 6e

Current Data Parameters
NAME INN-SOHAN-184D-1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150401
Time_ 15.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 54274
SOLVENT DMSO
NS 9
DS 0
SWH 8223.685 Hz
FIDRES 0.151522 Hz
AQ 3.2998593 sec
RG 32
DW 60.800 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 14.75 usec
PL1 -1.00 dB
PL1W 10.56200695 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

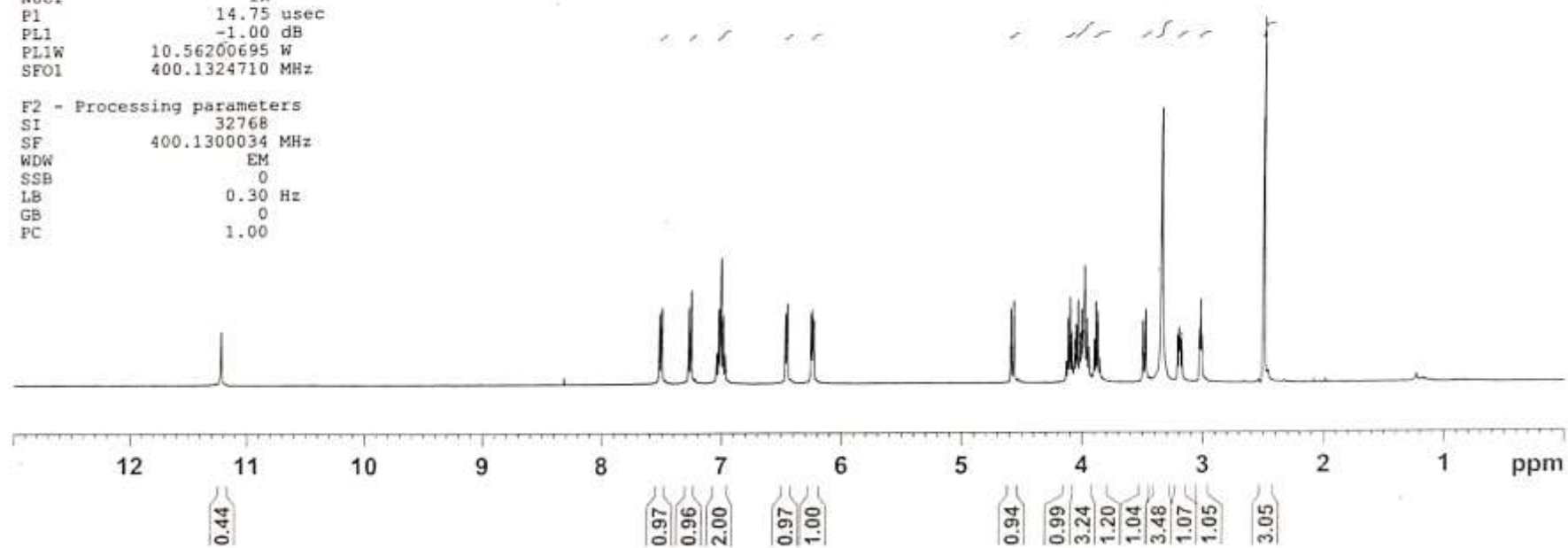
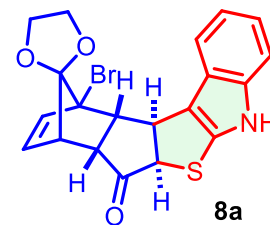


Figure S42. ¹H NMR of compound 8a

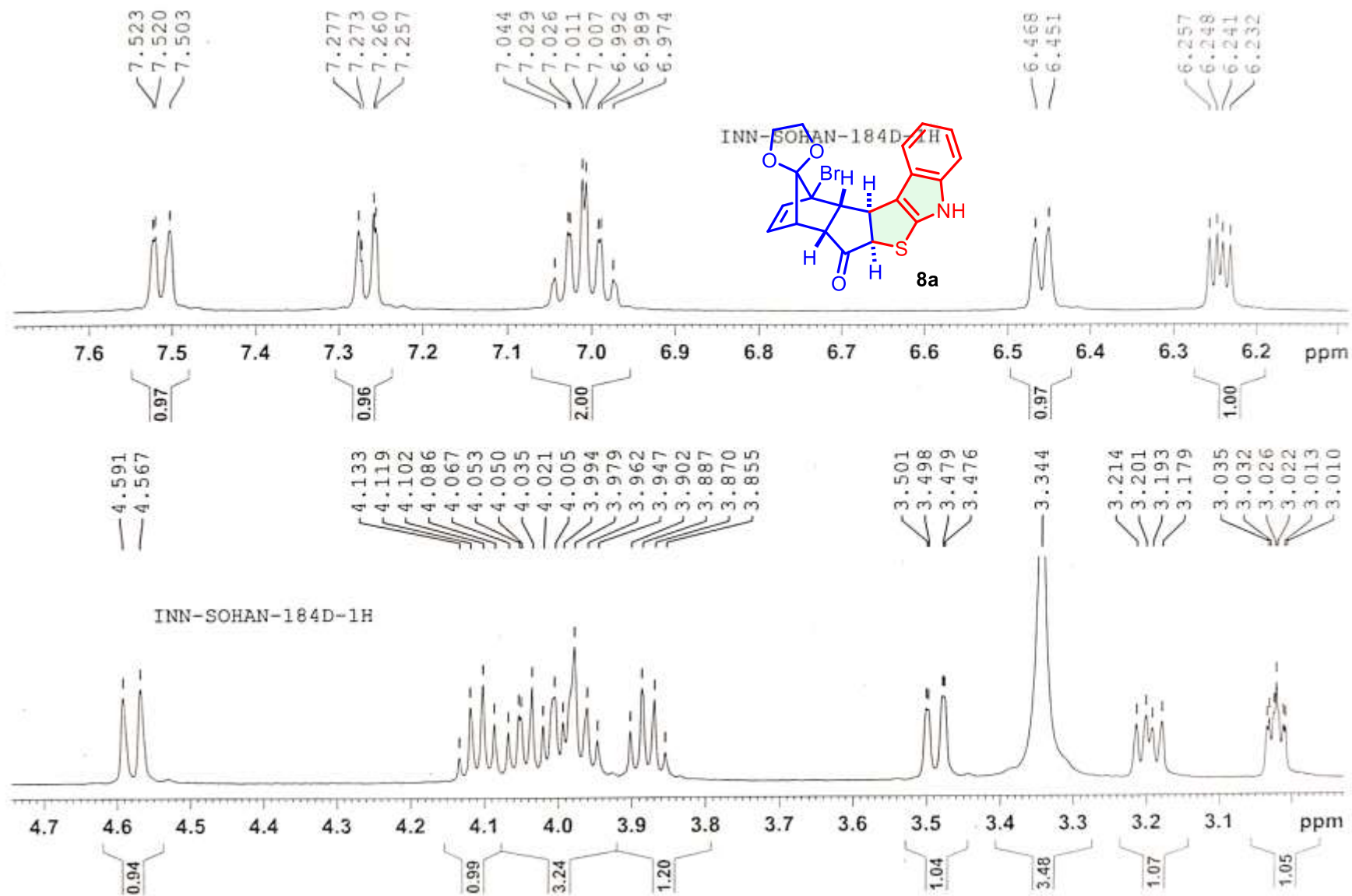


Figure S42a. Expansion of ^1H NMR of compound 8a

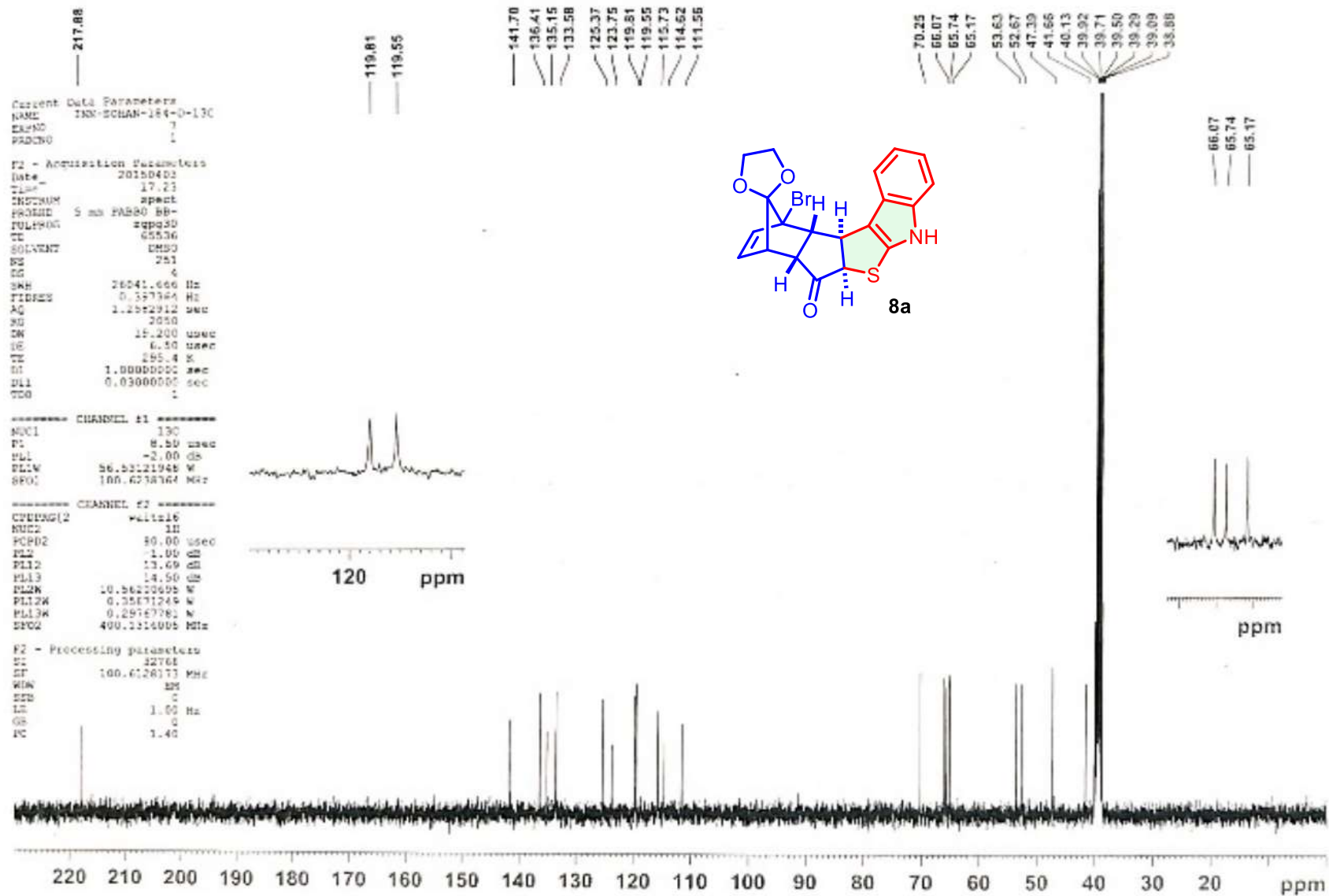


Figure S43. ¹³C NMR of compound **8a**

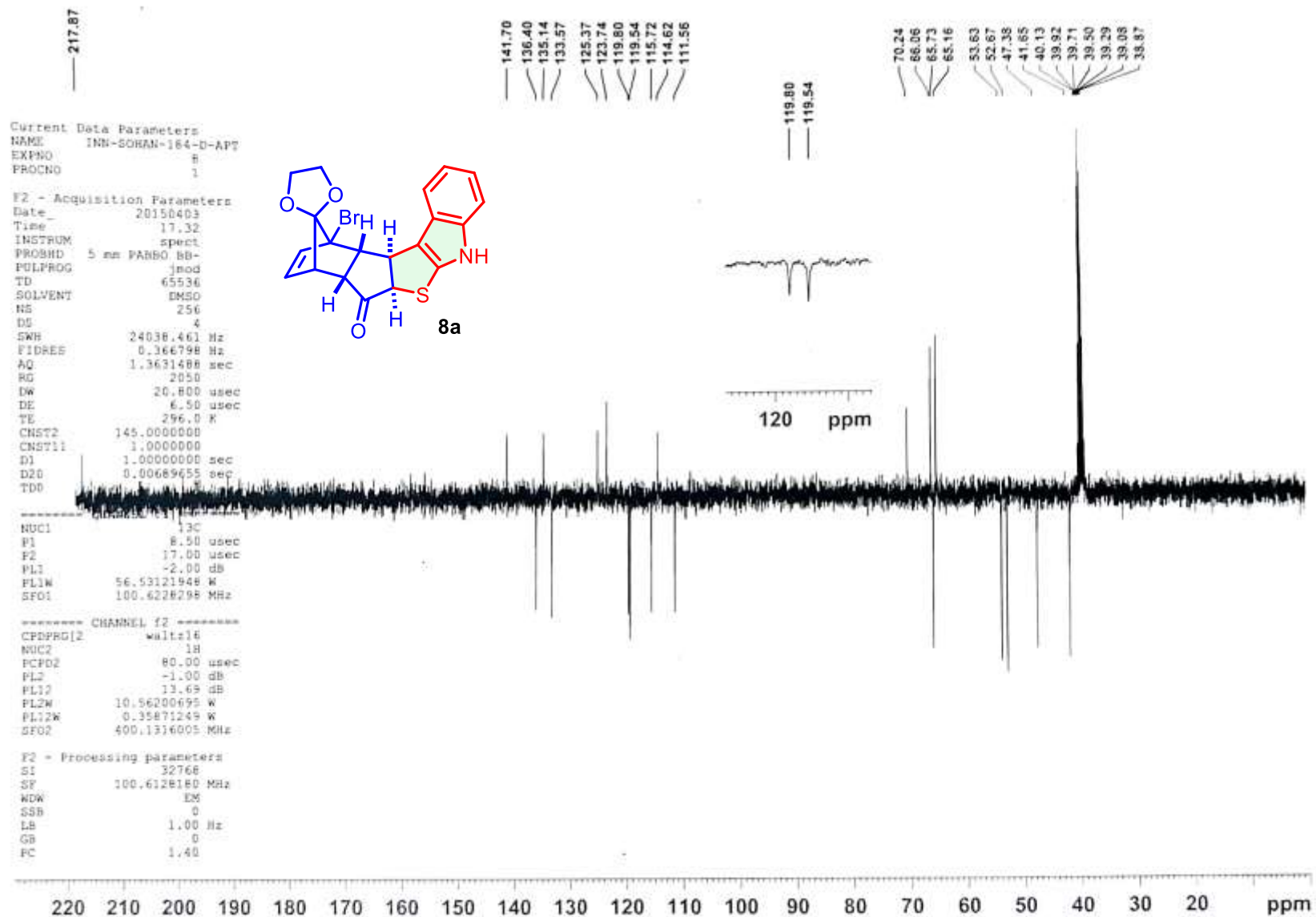


Figure S44. ¹³C-APT NMR of compound 8a

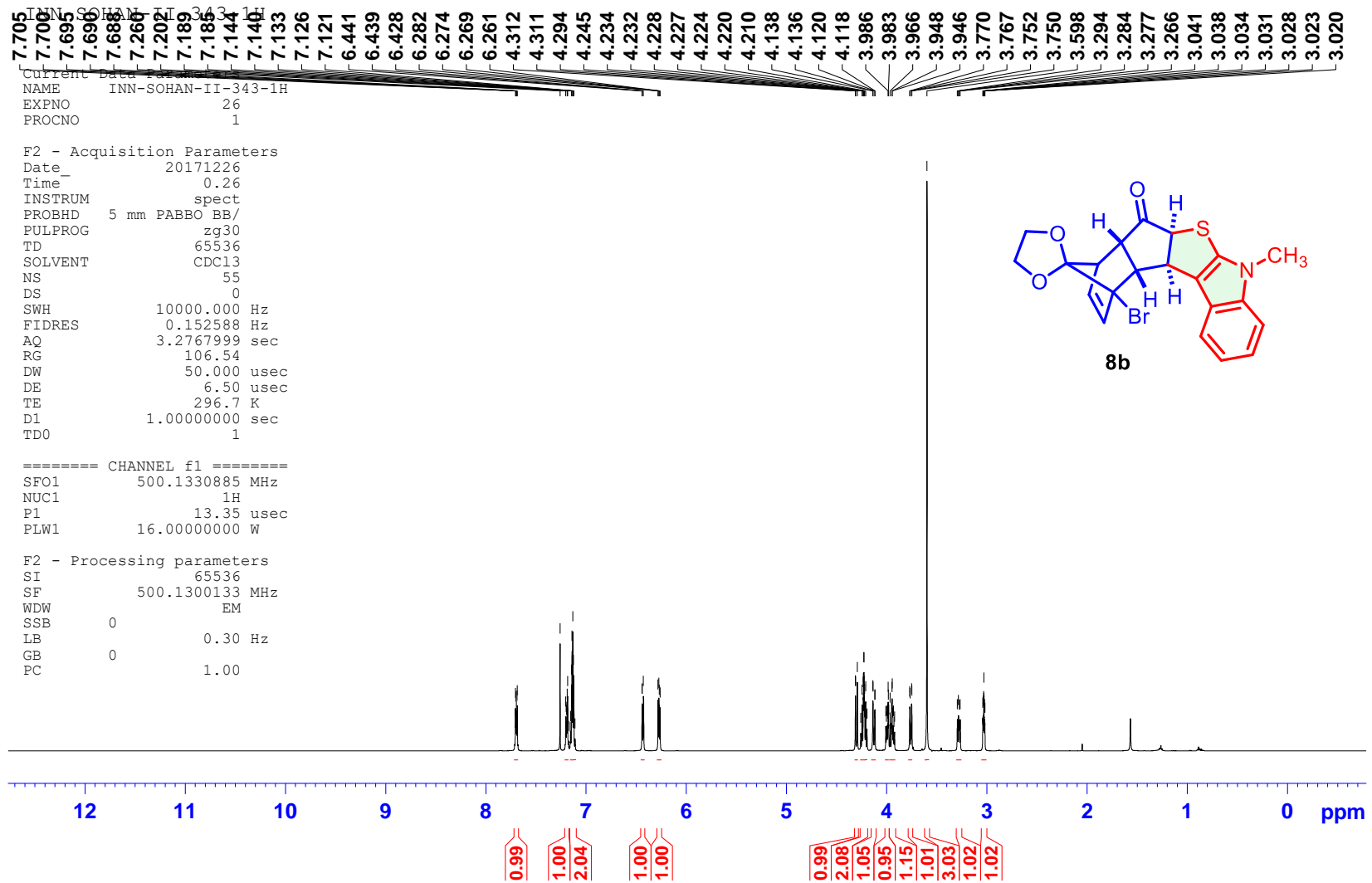


Figure S45. ¹H NMR of compound **8b**

INN-SOHAN-II-343-13C

Current Data Parameters
NAME INN-SOHAN-II-343-13C
EXPNO 27
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171226
Time_ 0.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 197.27
DW 15.000 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7716224 MHz
NUC1 13C
P1 8.90 usec
PLW1 103.00000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.44556001 W
PLW13 0.22411001 W

F2 - Processing parameters
SI 32768
SF 125.7577688 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

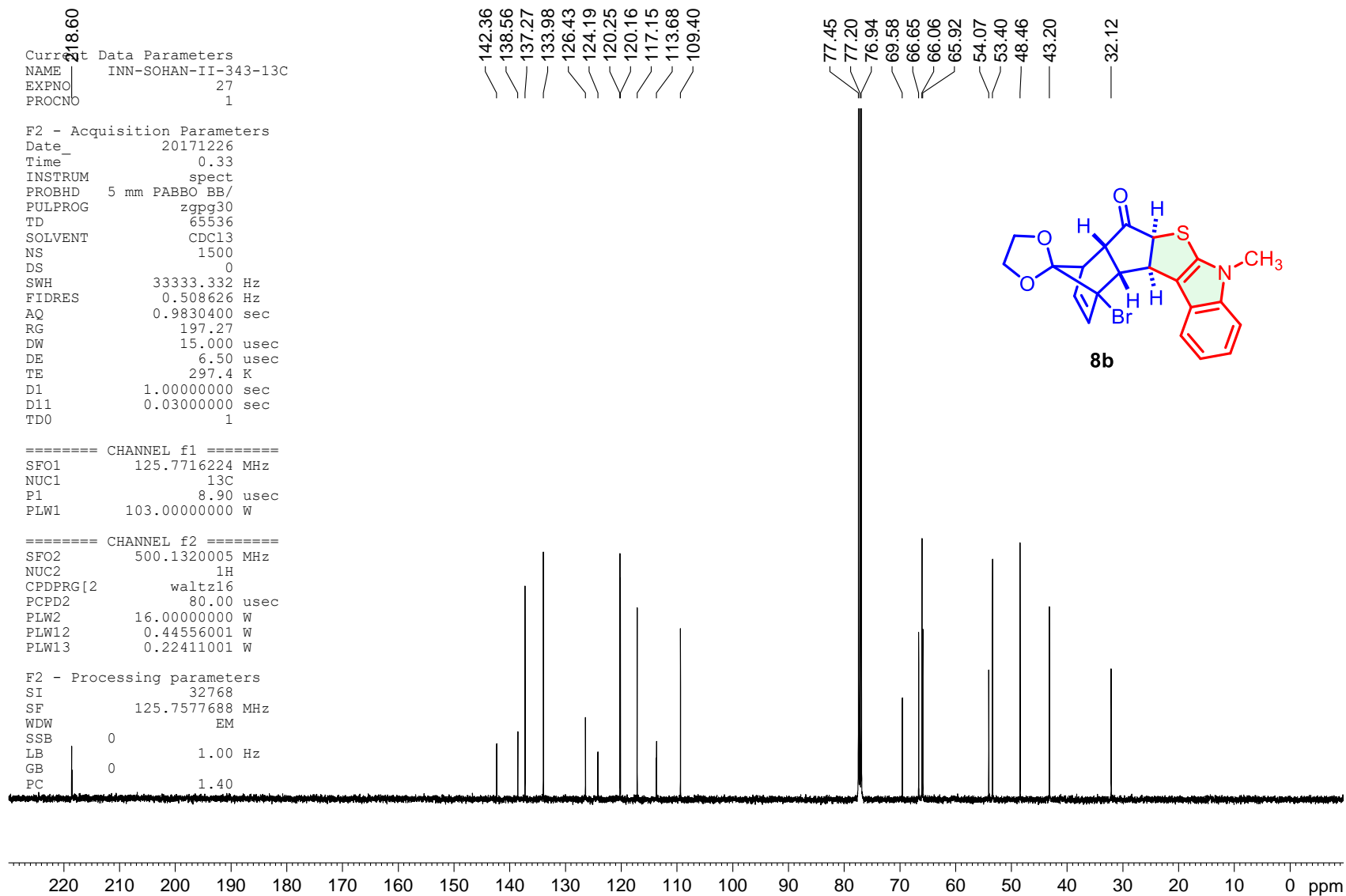


Figure S46. ¹³C NMR of compound 8b

INN-SOCHAN-II-343-APT

Current Data Parameters
NAME INN-SOCHAN-II-343-APT
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters

Date_ 20171226
Time 1.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1024
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 197.27
DW 15.000 usec
DE 6.50 usec
TE 298.6 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
D20 0.00689655 sec

==== CHANNEL f1 =====
SFO1 125.7716224 MHz
NUC1 13C
P1 8.90 usec
P2 17.80 usec
PLW1 103.00000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.44556001 W

F2 - Processing parameters
SI 32768
SF 125.7577666 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

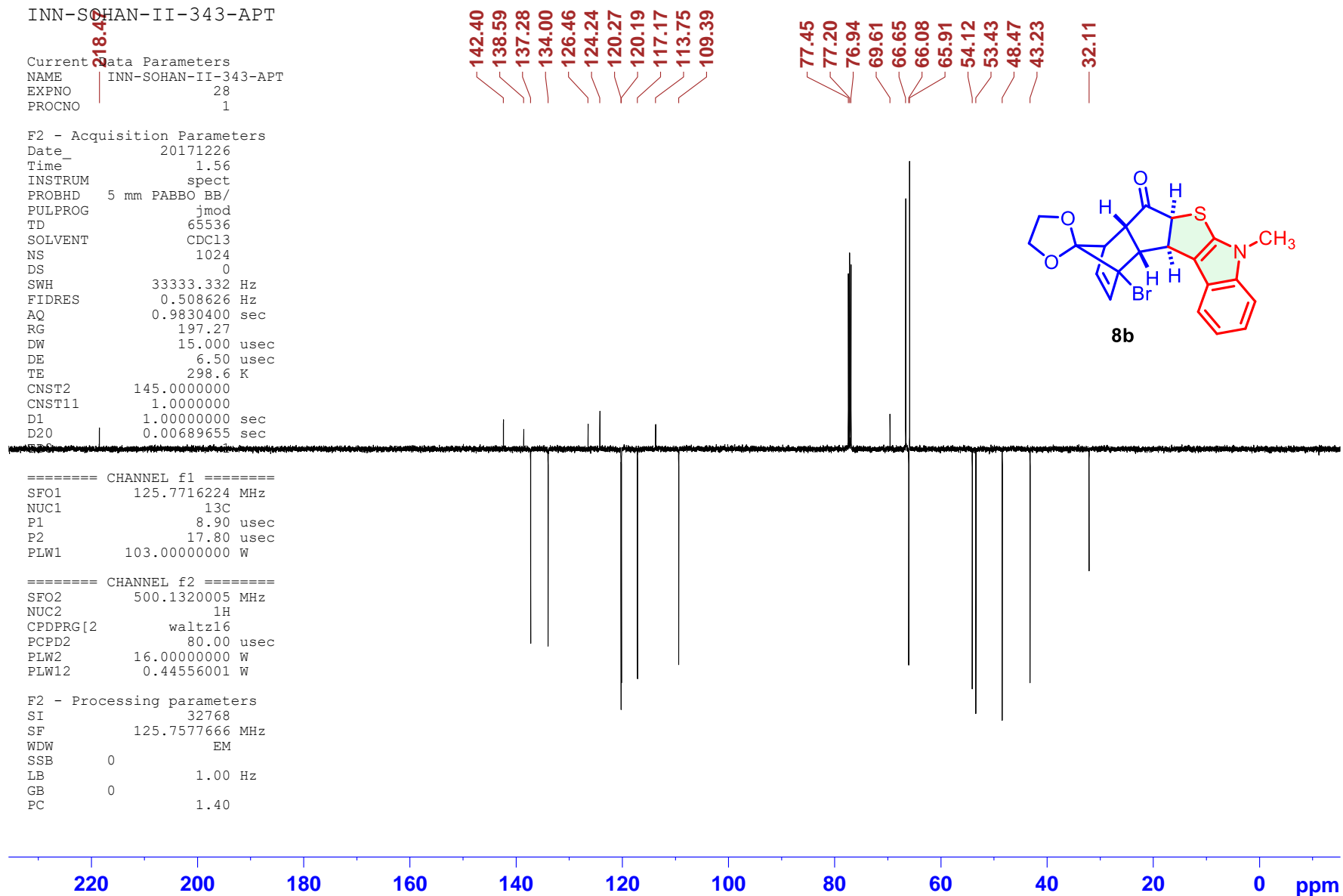


Figure S47. ¹³C-APT NMR of compound 8b

Current Data Parameters
NAME INN-DOHAH-II-343-COSY
EXPTNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171227
Time 14.57
INSTRUM spect
PROBHD 5 mm YAGBO BH-
PULPROG cosyppqf
TD 2048
SOLVENT CDCl3
NS 16
DS 0
SWH 2419.355 Hz
FIDRES 1.181326 Hz
AQ 0.4232533 sec
RG 640
DM 206.687 usec
DE 6.50 usec
TE 294.4 K
D0 0.00000300 sec
D1 1.00000000 sec
D12 0.00000400 sec
D16 0.00020000 sec
IN0 0.00041333 sec

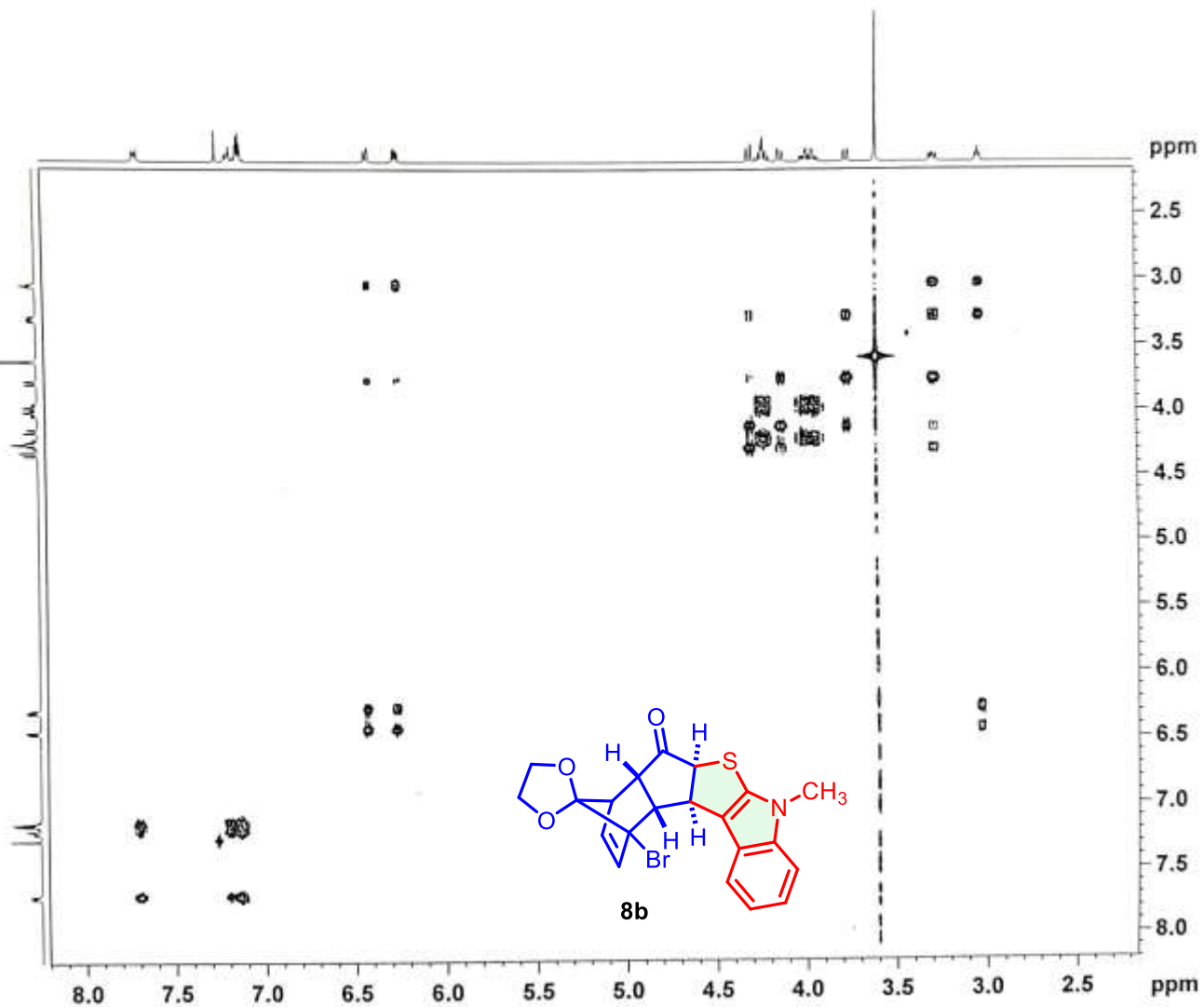
----- CHANNEL f1 -----
NUC1 1H
PC 14.75 usec
PI 14.75 usec
PL1 -1.00 dB
PS1W 10.56200695 W
SFO1 400.1300833 MHz

----- GRADIENT CHANNEL -----
GRAM(1) SINE.100
SP2 10.00 1
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.1321 MHz
FIDRES 18.901239 Hz
SW 6.046 ppm
FMODE CF

F2 - Processing parameters
SI 2048
SF 400.1300099 MHz
WDW SINC
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 512
MC2 CF
SF 400.1300099 MHz
WDW SINC
SSB 0
LB 0 Hz
GB 0



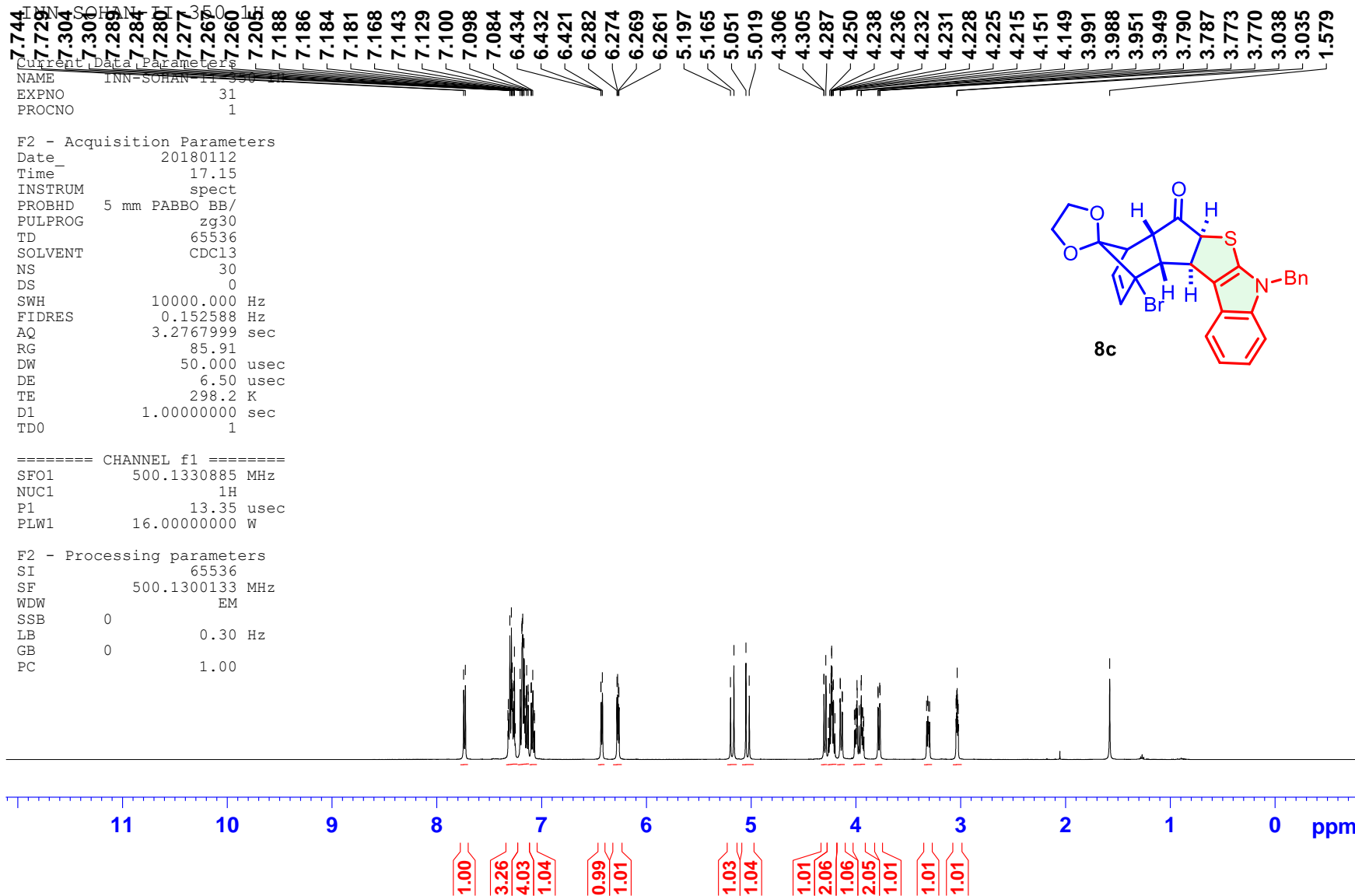


Figure S50. ¹H NMR of compound 8c

INN-SOCHAN-II-350-13C

Current Data Parameters
NAME INN-SOCHAN-II-350-13C
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180112
Time_ 17.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 414
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 197.27
DW 15.000 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 125.7716224 MHz
NUC1 13C
P1 8.90 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SF02 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.44556001 W
PLW13 0.22411001 W

F2 - Processing parameters
SI 32768
SF 125.7577713 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

141.95
138.18
137.19
136.44
134.02
128.98
128.08
127.49
126.42
124.41
120.45
120.38
117.27
114.56
109.93

77.45
77.20
76.94
69.60
66.63
66.24
65.90
54.04
53.43
49.72
48.42
43.06

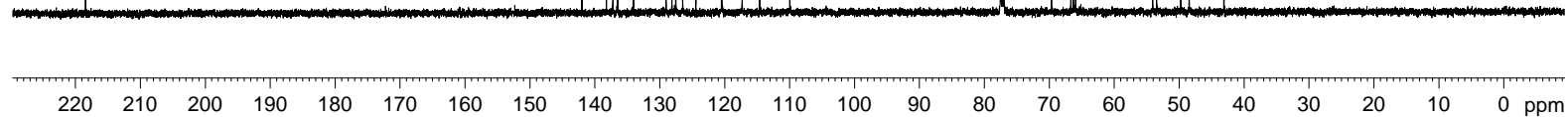
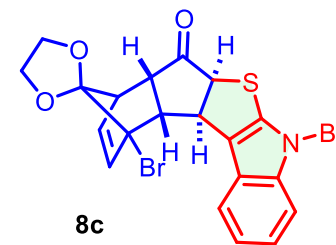


Figure S51. ¹³C NMR of compound 8c

INN-SOHAN-II-350-APT

Current Data Parameters
NAME INN-SOHAN-II-350-APT
EXPNO 33
PROCNO 1

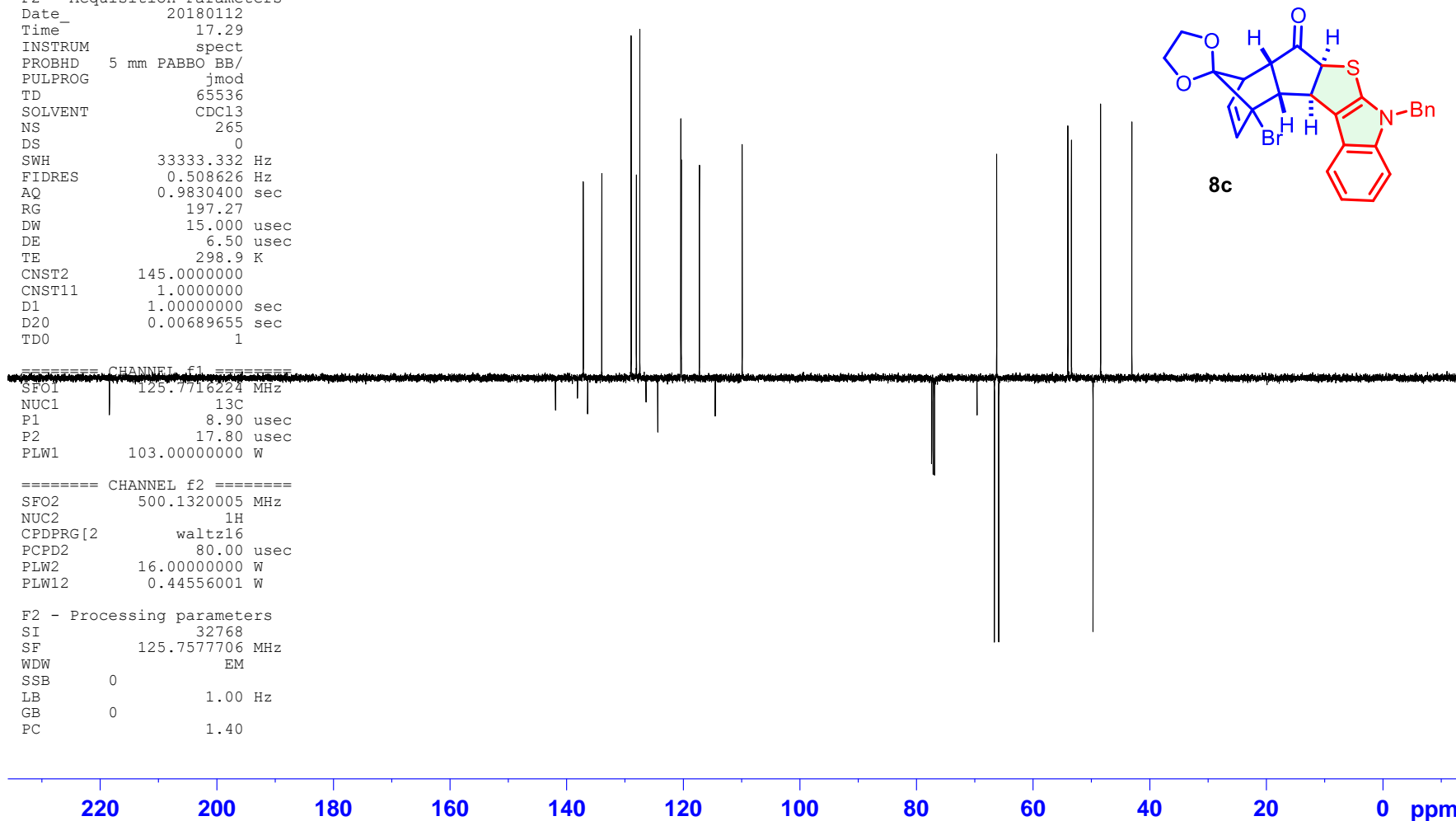
F2 - Acquisition Parameters
Date_ 20180112
Time_ 17.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG jmod
TD 65536
SOLVENT CDC13
NS 265
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 197.27
DW 15.000 usec
DE 6.50 usec
TE 298.9 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
D20 0.00689655 sec
TDO 1

===== CHANNEL f1 =====
SFO1 125.7716224 MHz
NUC1 13C
P1 8.90 usec
P2 17.80 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.44556001 W

F2 - Processing parameters
SI 32768
SF 125.7577706 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

141.96
138.19
137.19
136.45
134.02
128.98
128.09
127.49
126.43
124.42
120.46
120.38
117.27
114.56
109.94
77.45
77.20
76.94
69.61
66.63
66.25
65.90
54.04
53.43
49.72
48.42
43.07



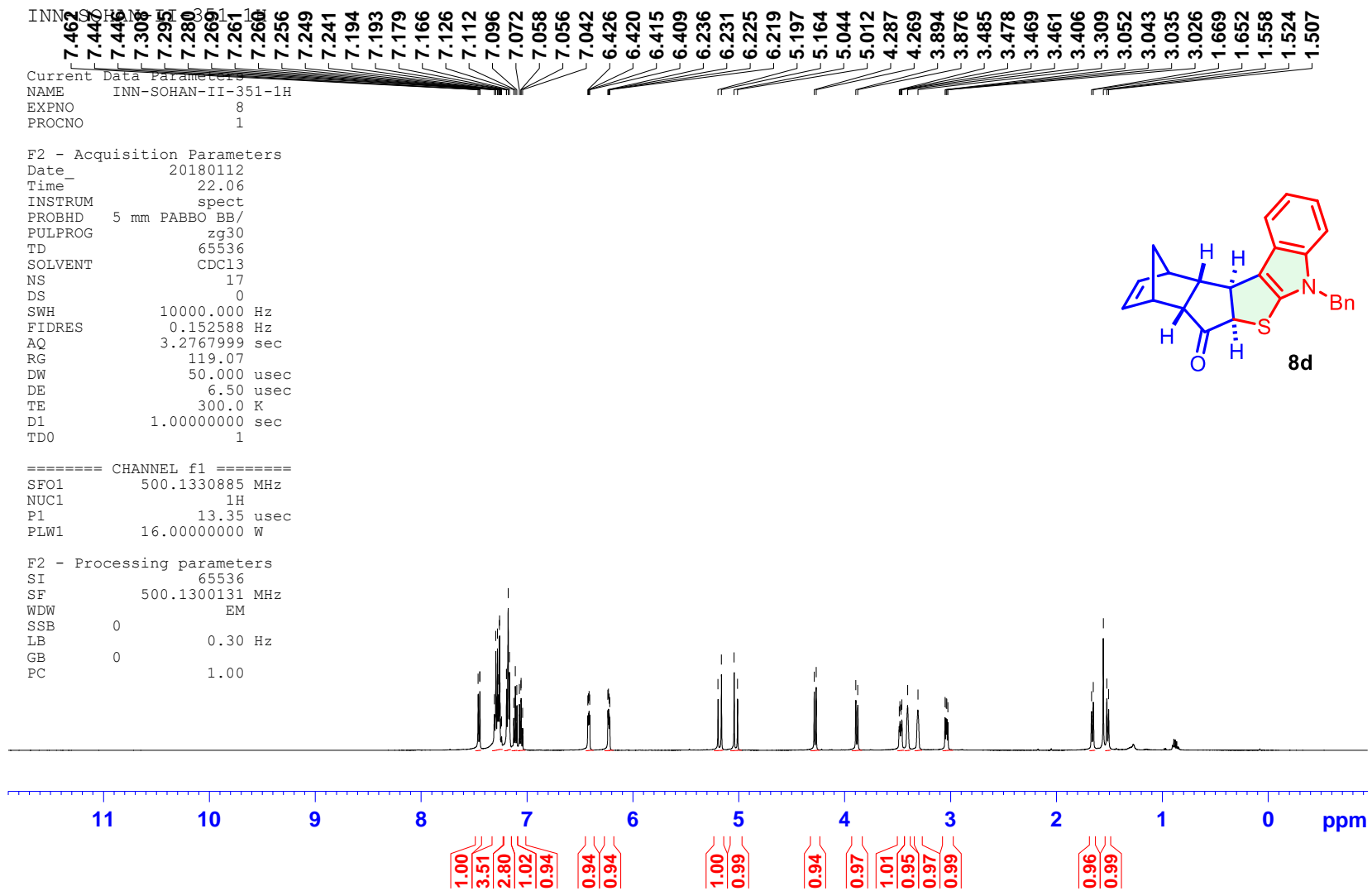


Figure S53. ¹H NMR of compound 8d

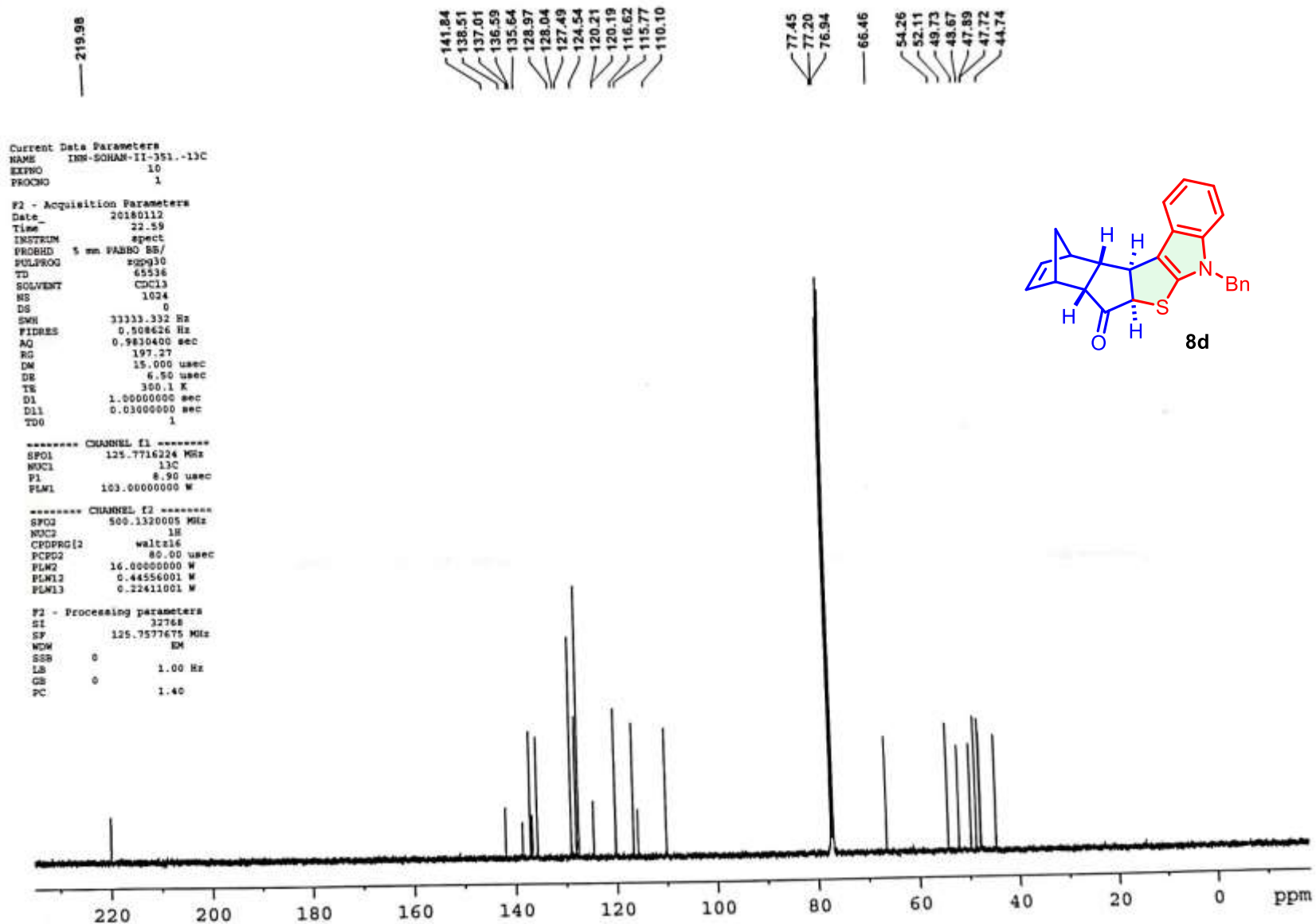


Figure S54. ¹³C NMR of compound 8d

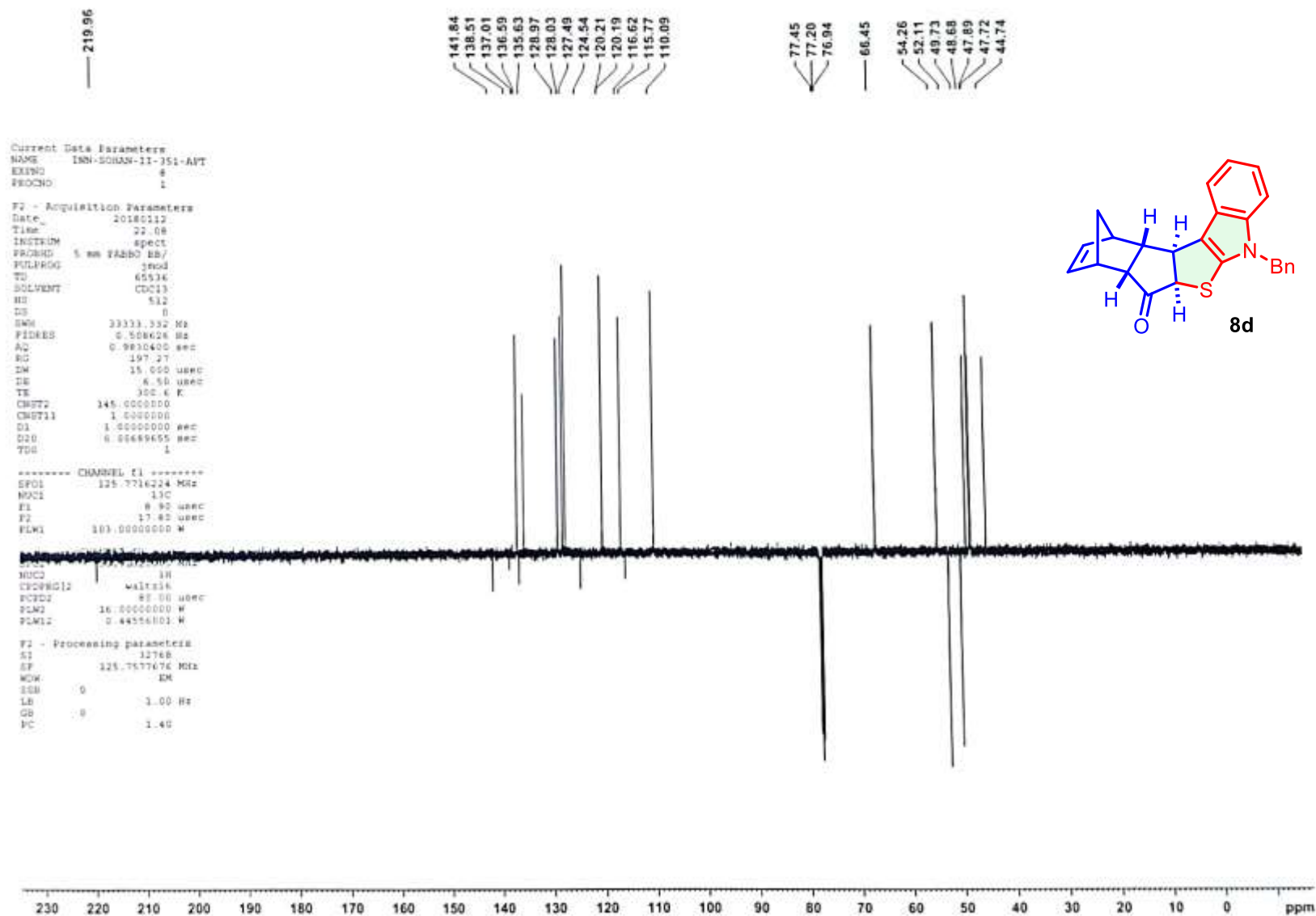
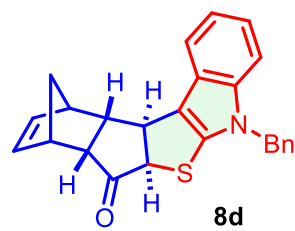


Figure S55. ¹³C-APT NMR of compound 8d



```

Current Data Parameters
NAME: INN-82448-11-101-COSY
EXPNO: 4
PROCNO: 1

F2 - Acquisition Parameters
Date_ : 20100114
Time: 11.26
INSTRUM: spect
PROBHD: 5 mm TANGO BB/
PULPROG: zgpg30
TD: 6548
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 3388.821 Hz
FIDRES: 1.751247 Hz
AQ: 0.2854932 sec
RG: 197.17
IN: 330.400 MHz
DE: 4.00 MHz
TE: 300.0 K
D0: 0.0002000 sec
D1: 1.2000000 sec
d11: 0.0000000 sec
d12: 0.0000000 sec
d13: 0.0000000 sec
d14: 0.0000000 sec
d15: 0.0002000 sec
d16: 0.0002000 sec
d17: 0.0002000 sec
----- CHANNEL f1 -----
SFO1: 500.1323609 MHz
NUC1: 1H
P1: 13.00 MHz
P2: 13.00 MHz
PCY: 2500.00 MHz
TIM1: 14.0000000 W
FAM1B: 3.3680000 W
----- CHANNEL f2 -----
CHAN(f2): 500.1323609 MHz
CPC1: 18.00 MHz
P1c: 1000.00 MHz
F1 - Acquisition parameters
TD: 6548
SFO1: 500.1323609 MHz
FIDRES: 1.751247 Hz
IN: 330.400 MHz
PULPROG: zgpg30
F2 - Processing parameters
SI: 32768
SF: 500.1323609 MHz
WDW: EM
GB: 0
LB: 0 Hz
GB: 0
PC: 1.40
F3 - Processing parameters
SI: 1324
SF: 500.1323609 MHz
WDW: EM
GB: 0
LB: 0 Hz
GB: 0

```

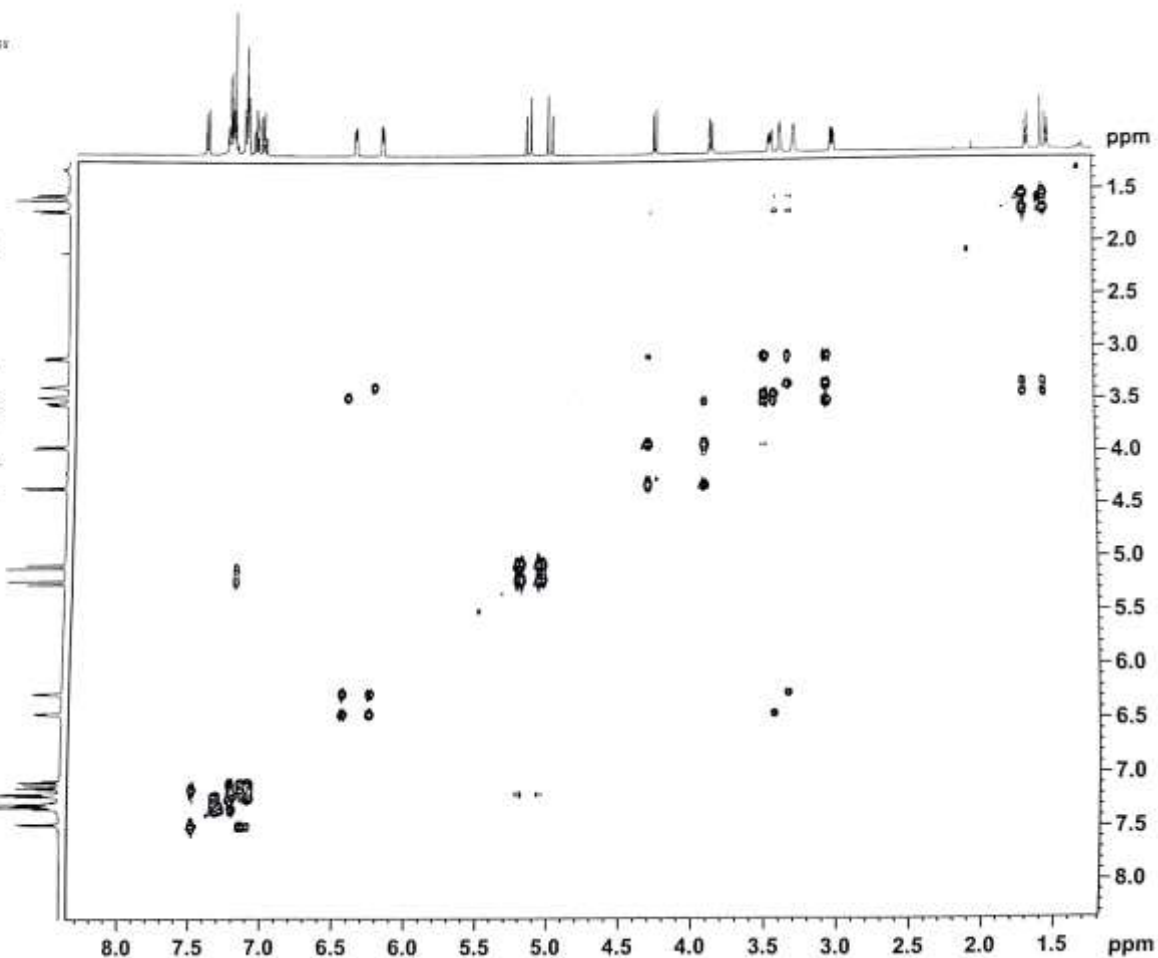
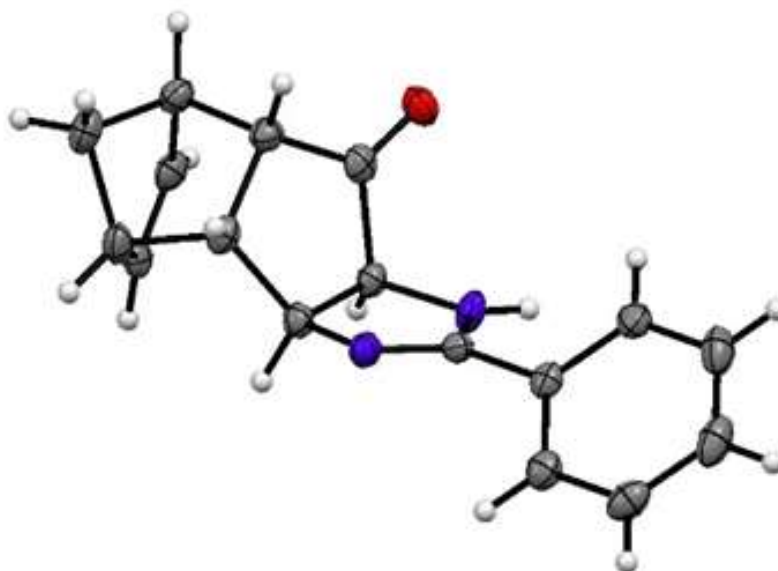
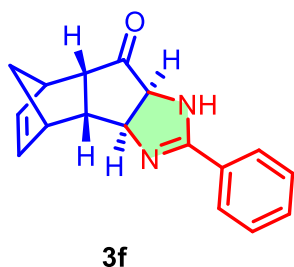


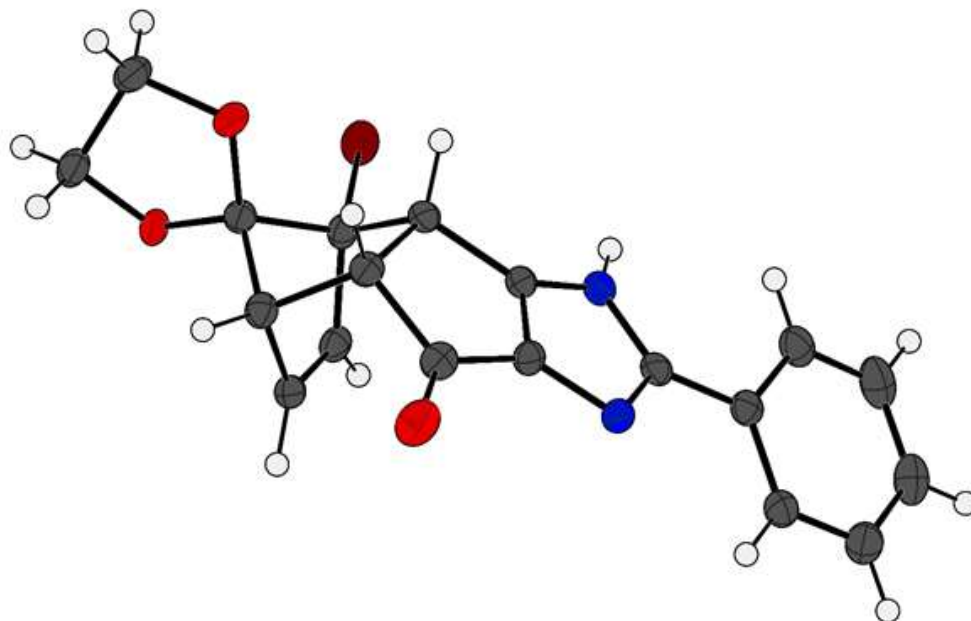
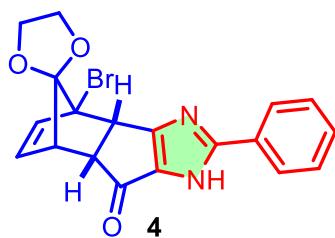
Figure S56. ^1H - ^1H COSY NMR of compound 8d

Table S1. Crystal data and structure refinement for CCDC 1974406 (3f)



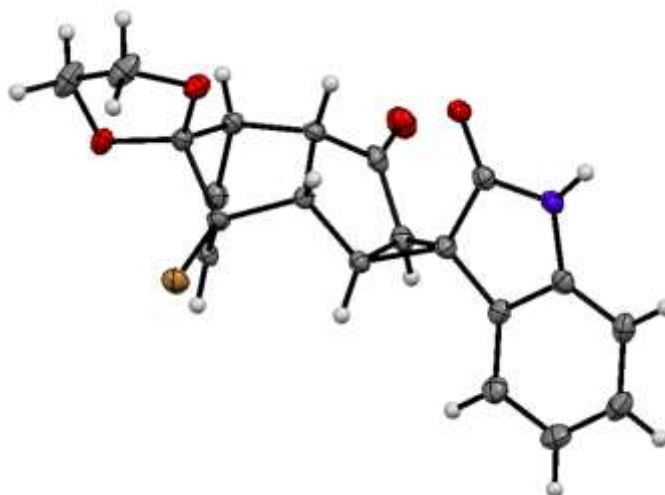
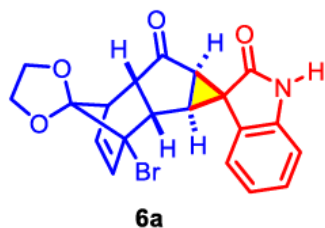
Identification code	INN-SOHAN-II-29
Empirical formula	C ₁₇ H ₁₆ N ₂ O
Formula weight	264.32
Temperature/K	150
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	9.5078(8)
b/Å	11.2634(9)
c/Å	12.0926(10)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	1295.00(18)
Z	4
ρ _{calc} /cm ³	1.356
μ/mm ⁻¹	0.086
F(000)	560.0
Crystal size/mm ³	0.223 × 0.126 × 0.102
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.942 to 49.986
Index ranges	-8 ≤ h ≤ 11, -13 ≤ k ≤ 7, -14 ≤ l ≤ 14
Reflections collected	7151
Independent reflections	2283 [R _{int} = 0.0540, R _{sigma} = 0.0551]
Data/restraints/parameters	2283/0/181
Goodness-of-fit on F ²	1.074
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0441, wR ₂ = 0.0942
Final R indexes [all data]	R ₁ = 0.0532, wR ₂ = 0.1008
Largest diff. peak/hole / e Å ⁻³	0.21/-0.20

Table S2. Crystal data and structure refinement for CCDC 2530978 (4)



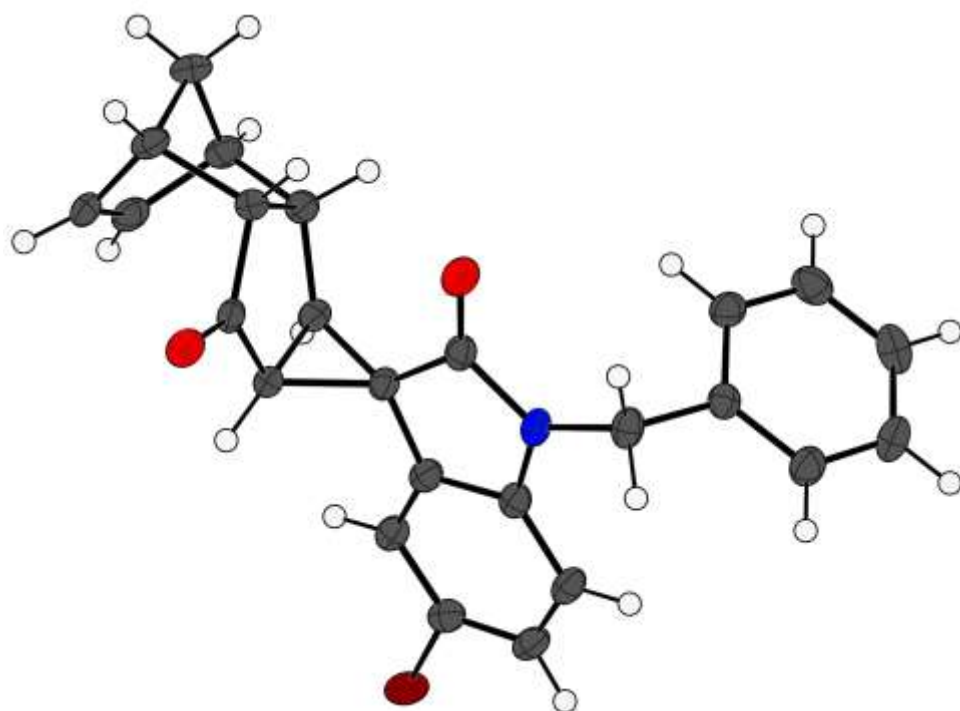
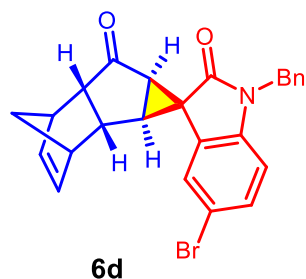
Identification code	INN_TGL_04_56_autored
Empirical formula	C ₂₁ H ₂₁ BrN ₂ O ₄ S
Formula weight	477.37
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.4144(4)
b/Å	9.5780(4)
c/Å	12.3679(5)
α/°	111.479(4)
β/°	95.220(3)
γ/°	101.940(3)
Volume/Å ³	998.15(8)
Z	2
ρ _{calc} /cm ³	1.588
μ/mm ⁻¹	2.195
F(000)	488.0
Crystal size/mm ³	0.15 × 0.13 × 0.11
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	3.6 to 49.988
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -14 ≤ l ≤ 14
Reflections collected	35607
Independent reflections	3515 [R _{int} = 0.0999, R _{sigma} = 0.0375]
Data/restraints/parameters	3515/0/227
Goodness-of-fit on F ²	1.059
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0373, wR ₂ = 0.1003
Final R indexes [all data]	R ₁ = 0.0403, wR ₂ = 0.1031
Largest diff. peak/hole / e Å ⁻³	0.74/-0.77

Table S3. Crystal data and structure refinement for CCDC 1974453 (6a)



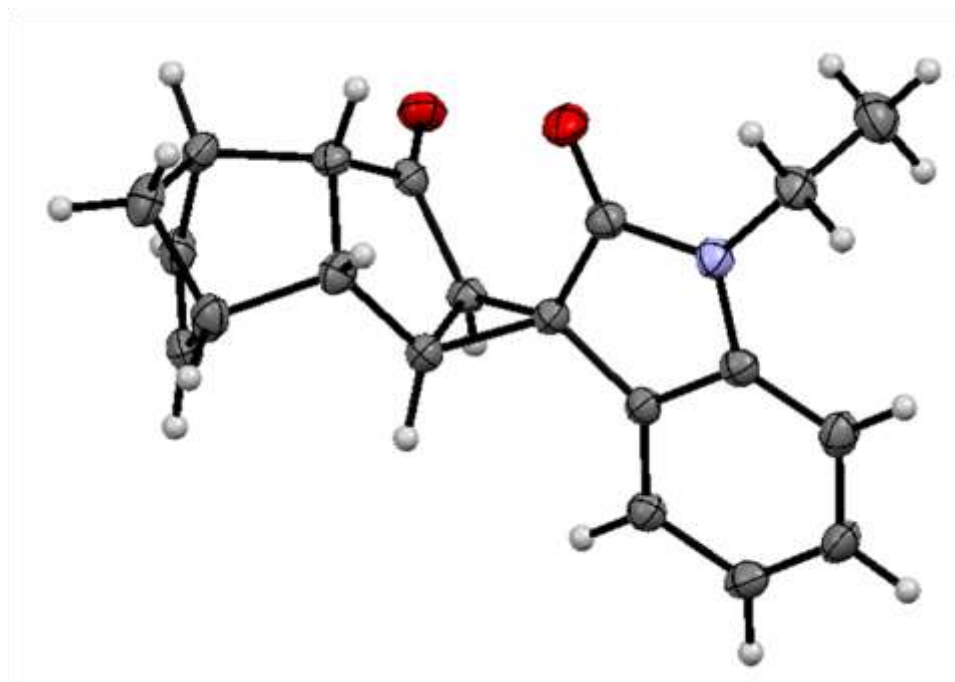
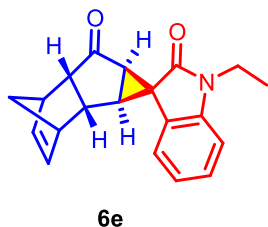
Identification code	INN-SOHAN-II-251-B
Empirical formula	C ₂₀ H ₁₆ BrNO ₄
Formula weight	414.25
Temperature/K	150
Crystal system	monoclinic
Space group	P2 ₁ /c
a / Å	12.1893
b / Å	6.7861
c / Å	20.6372
α / °	90
β / °	93.489
γ / °	90
Volume/Å ³	1703.90
Z	4
ρ _{calc} g/cm ³	1.615
μ / mm ⁻¹	2.439
F(000)	840.0
Crystal size/mm ³	0.207 × 0.12 × 0.04
Radiation	MoKα (λ = 0.71073)
2θ range for data collection	5.024 to 49.99°
Index ranges	-14 ≤ h ≤ 14, -8 ≤ k ≤ 6, -23 ≤ l ≤ 24
Reflections collected	14616
Independent reflections	2997 [R _{int} = 0.0562, R _{sigma} = 0.0378]
Data/restraints/parameters	2997/0/235
Goodness-of-fit on F ²	1.044
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0328, wR ₂ = 0.0717
Final R indexes [all data]	R ₁ = 0.0400, wR ₂ = 0.0756
Largest diff. peak/hole / e Å ⁻³	0.36/-0.41

Table S4. Crystal data and structure refinement for CCDC 1974434 (6d)



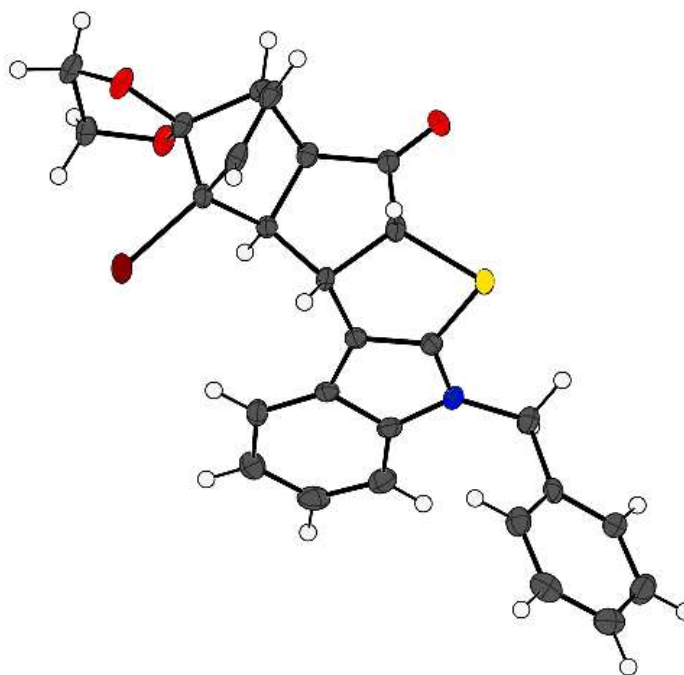
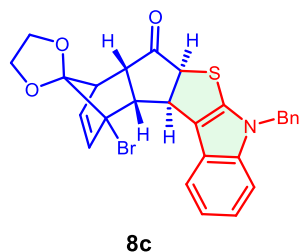
Identification code	INN-SOHAN-II-300
Empirical formula	C ₂₅ H ₂₀ BrNO ₂
Formula weight	446.33
Temperature/K	150
Crystal system	triclinic
Space group	P-1
a/Å	8.7539(3)
b/Å	10.9118(4)
c/Å	12.2664(3)
α/°	66.662(3)
β/°	87.517(2)
γ/°	68.820(3)
Volume/Å ³	996.32(6)
Z	2
ρ _{calc} /g/cm ³	1.488
μ/mm ⁻¹	2.085
F(000)	456.0
Crystal size/mm ³	0.24 × 0.18 × 0.124
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	5.696 to 49.986
Index ranges	-10 ≤ h ≤ 8, -12 ≤ k ≤ 12, -14 ≤ l ≤ 14
Reflections collected	7281
Independent reflections	3478 [R _{int} = 0.0667, R _{sigma} = 0.0556]
Data/restraints/parameters	3478/0/262
Goodness-of-fit on F ²	1.062
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0385, wR ₂ = 0.0978
Final R indexes [all data]	R ₁ = 0.0438, wR ₂ = 0.1013
Largest diff. peak/hole / e Å ⁻³	1.41/-0.41

Table S5. Crystal data and structure refinement for CCDC 1992116 (6e)



Identification code	INN-SOHAN-II-330_Mo
Empirical formula	C ₂₀ H ₁₉ NO ₂
Formula weight	305.379
Temperature/K	150.00
Crystal system	triclinic
Space group	P-1
a/Å	8.3696(4)
b/Å	9.9170(4)
c/Å	20.0570(9)
α/°	96.597(3)
β/°	94.003(4)
γ/°	112.839(4)
Volume/Å ³	1512.14(12)
Z	4
ρ _{calc} /cm ³	1.341
μ/mm ⁻¹	0.086
F(000)	648.4
Crystal size/mm ³	0.24 × 0.18 × 0.12
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.66 to 50
Index ranges	-12 ≤ h ≤ 10, -14 ≤ k ≤ 14, -27 ≤ l ≤ 23
Reflections collected	15873
Independent reflections	5295 [R _{int} = 0.0469, R _{sigma} = 0.0690]
Data/restraints/parameters	5295/0/417
Goodness-of-fit on F ²	1.058
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0444, wR ₂ = 0.0986
Final R indexes [all data]	R ₁ = 0.0572, wR ₂ = 0.1064
Largest diff. peak/hole / e Å ⁻³	0.35/-0.39

Table S6. Crystal data and structure refinement for CCDC 1992303 (8c)



Identification code	INN-SOHAN-II-350_Mo
Empirical formula	C ₂₇ H ₂₂ BrNO ₃ S
Formula weight	520.42
Temperature/K	150
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	10.4378(5)
b/Å	10.0604(4)
c/Å	21.4824(10)
α/°	90
β/°	101.308(5)
γ/°	90
Volume/Å ³	2212.04(18)
Z	4
ρ _{calc} /cm ³	1.563
μ/mm ⁻¹	1.984
F(000)	1064.0
Crystal size/mm ³	0.123 × 0.113 × 0.078
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.976 to 49.996
Index ranges	-11 ≤ h ≤ 12, -11 ≤ k ≤ 11, -25 ≤ l ≤ 24
Reflections collected	11757
Independent reflections	3886 [R _{int} = 0.0414, R _{sigma} = 0.0477]
Data/restraints/parameters	3886/0/298
Goodness-of-fit on F ²	1.024
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0365, wR ₂ = 0.0745
Final R indexes [all data]	R ₁ = 0.0482, wR ₂ = 0.0812
Largest diff. peak/hole / e Å ⁻³	0.36/-0.40

Table S7. Cartesian coordinates for the optimized geometries at B3LYP/6-31G(d) (solvent model, MeCN) level of theory (All energies are reported in Hartrees)

1				TS-(1+5)			
E = -3033.405557				E = -3471.990935			
G = -3033.276282				G = -3471.751295			
C	1.19125000	-0.83919900	-0.78604500	C	1.79119800	-0.93961800	-0.98173800
C	2.25217000	-1.26007200	0.30693800	C	2.19608500	-2.09567400	0.00765000
C	2.22721500	0.99680000	0.46726500	C	3.73452100	-0.50464800	0.47076200
C	1.17681100	0.71589400	-0.67270600	C	2.88453500	0.14000700	-0.67627100
H	1.49114500	-1.20629600	-1.77397900	H	1.83946300	-1.30327400	-2.01484000
H	1.44641400	1.23272300	-1.59906700	H	3.51524700	0.35192800	-1.54844600
C	1.97579700	-0.20798400	1.40783300	C	2.63889800	-1.27690000	1.24665000
H	2.70097000	-0.25830200	2.22520400	H	3.05082800	-1.90740900	2.04222500
H	0.96340400	-0.25037600	1.82389400	H	1.85370300	-0.63357000	1.65538400
C	3.58677200	-0.74659900	-0.22649300	C	3.55021400	-2.60434800	-0.48102500
H	4.34714600	-1.36906000	-0.68819800	H	3.69643900	-3.52017000	-1.04696900
C	3.57068100	0.59331500	-0.13341200	C	4.46732100	-1.66490400	-0.19557000
H	4.31353700	1.29240400	-0.50538800	H	5.51498600	-1.65515000	-0.48364800
H	2.21111000	-2.31463800	0.58769300	H	1.43836300	-2.86886400	0.14476300
H	2.15962400	2.00007400	0.89212300	H	4.34778400	0.20541100	1.03039500
C	-0.26110500	1.07931100	-0.31571200	C	2.11938200	1.42434100	-0.34947600
C	-0.22714500	-1.24835000	-0.49585100	C	0.44818700	-0.20361100	-0.81437600
H	-0.54818200	-2.28566300	-0.49147900	C	0.74622400	1.13958500	-0.55501400
C	-1.02088400	-0.19132400	-0.24941300	O	2.67420400	2.50839500	-0.05480300
O	-0.69742400	2.20602700	-0.12461900	Br	-0.57863700	2.51671200	-0.54379900
Br	-2.86671800	-0.22399500	0.13462100	C	-4.74866200	-1.25103000	-0.80265100
5				C	-4.35018000	-0.36264100	0.21162200
E = -438.600176				C	-3.03675200	-0.43718300	0.66357000
G = -438.511992				C	-2.10094200	-1.37296400	0.13732900
C	2.52732100	-0.74926600	0.00004600	C	-2.52135100	-2.24388100	-0.87524800
C	1.29202600	-1.42303500	0.00007300	C	-3.84690800	-2.18251100	-1.33605500
C	0.12520800	-0.66424600	0.00000300	H	-5.77004500	-1.21237300	-1.17339500
C	0.13780500	0.77380600	-0.00004300	H	-5.04974600	0.35739900	0.62967000
C	1.39186800	1.41825900	-0.00003000	H	-1.82985300	-2.96922100	-1.29964200
C	2.56856900	0.65626600	-0.00000400	H	-4.17537100	-2.86267000	-2.11846200
H	3.45203600	-1.32165600	0.00008100	C	-0.81606200	-1.12425800	0.77104800
H	1.25132300	-2.51081400	0.00010600	C	-1.05398900	-0.10789000	1.78937400
H	1.44833200	2.50584200	-0.00000900	N	-2.39016400	0.29124800	1.65659700
H	3.53196100	1.16308900	0.00000900	H	-2.77201100	1.09279500	2.14082500
C	-1.22282200	1.21182900	0.00008100	O	-0.27524200	0.39239400	2.62814300
H	-1.58010900	2.23494300	0.00026600	H	-0.37403000	-0.48524400	-1.46301400
C	-2.06510400	0.07472100	-0.00019900	H	-0.10431200	-1.91079000	0.97174000
N	-1.20368000	-1.05178100	-0.00005700	TS-XVIIa			
H	-1.54522200	-2.00308300	0.00017000	E = -3471.994710			
O	-3.33272400	-0.06198300	0.00002700	G = -3471.750818			
Intermediate (1+5)				C	-0.96224900	1.07499100	-0.94490800
E = -3472.024599				C	-0.06813800	2.36257400	-1.02449000
G = -3471.782602				C	-1.29944300	2.76624800	0.83405700
C	-1.06017400	1.26371600	-0.75578600	C	-1.76113500	1.34763300	0.38121100
C	-1.07235200	2.35927800	0.37236100	H	-1.63469800	1.06000700	-1.80505600
C	-3.25571900	1.79223400	0.23215900	H	-2.84474900	1.31223400	0.23138000
C	-2.56172800	0.83936200	-0.82517700	C	0.19632100	2.67386100	0.47687600
H	-0.71461700	1.71651500	-1.68895200	H	0.73592400	3.61509400	0.62536600
H	-3.03428500	0.94096700	-1.80759400	H	0.70534500	1.87374900	1.02234200
C	-2.16994600	1.83912900	1.33329900	C	-1.04418300	3.49480000	-1.34676100
H	-2.41126900	2.56039700	2.12070800	H	-1.17316900	3.93092000	-2.33326600
H	-1.93766700	0.87598600	1.79519400	C	-1.78095600	3.72788200	-0.24826900
C	-1.81639900	3.53823900	-0.24809500	H	-2.63102700	4.39704400	-0.15160600
H	-1.34124900	4.43040900	-0.64638600	H	0.78597800	2.28175300	-1.69840200
C	-3.11386800	3.19772400	-0.34038200	H	-1.55876800	3.01481000	1.86536000
H	-3.91289600	3.75075600	-0.82544600	C	-1.41289400	0.17775300	1.29181000
H	-0.08909100	2.56967300	0.79613500	C	-0.36755900	-0.38228700	-0.84876200
H	-4.26227400	1.47544500	0.51431700	C	-0.95515500	-0.93353400	0.41313700
C	-2.61044600	-0.62518500	-0.41900400	O	-1.54467700	0.12921300	2.51115700
C	-0.22744300	-0.05802000	-0.52503900	Br	-3.27673500	-1.67226600	-0.11312700
C	-1.23802700	-1.04024300	0.08802200	C	5.11921700	0.24805200	0.41750400
O	-3.59775800	-1.33904100	-0.48961900	C	4.61514000	-1.05753900	0.38193300
C	5.09935300	0.78340100	-0.83258600	C	3.26842000	-1.23740900	0.08559600
C	4.67833600	0.49049100	0.47755600	C	2.35185200	-0.15979800	-0.15938500
C	3.32333400	0.26655800	0.70079100	C	2.91567200	1.13396400	-0.15434100
C	2.34759000	0.32682000	-0.35094200	C	4.27124200	1.32715600	0.13571700
				H	6.16839800	0.41795900	0.64456300
				H	5.25859400	-1.91498400	0.56362900
				H	2.32563200	2.00401800	-0.39251400

C	2.79957400	0.62621900	-1.65227700
C	4.16485100	0.84843200	-1.88082400
H	6.15372600	0.96102400	-1.03103100
H	5.39561800	0.43613800	1.29439600
H	2.09465800	0.68903400	-2.47977600
H	4.50637700	1.07796200	-2.88852700
C	1.06665500	0.04198900	0.22258200
C	1.25467300	-0.19429200	1.60877600
N	2.63849700	-0.04435600	1.86136700
H	3.04560100	-0.17224200	2.77769900
O	0.43911000	-0.49615600	2.54307600
H	-0.00979200	-0.42235800	-1.54015900
H	-1.19800900	-0.99285500	1.18156100
Br	-0.83242100	-2.93371100	-0.29319900

TS-XVIa
E = -3471.999704
G = -3471.756754

C	-0.83156100	0.86484000	-0.91735400
C	0.03949100	2.15936600	-0.74510700
C	-1.74106100	2.60616700	0.57526200
C	-2.05409800	1.17056600	0.01352500
H	-1.13997300	0.75863200	-1.96024100
H	-3.01441900	1.16282100	-0.51024700
C	-0.20605300	2.51629000	0.74347700
H	0.24228400	3.47572000	1.02248500
H	0.11006600	1.74338200	1.44783200
C	-0.76352800	3.27283800	-1.41373400
H	-0.55584100	3.68001600	-2.39942900
C	-1.82436200	3.53619200	-0.63119800
H	-2.65747400	4.19944700	-0.84601600
H	1.07553900	2.04730400	-1.07010100
H	-2.33665400	2.87963400	1.44907700
C	-2.10233000	0.05816200	1.05685800
C	-0.19685700	-0.51031200	-0.44846300
C	-1.10972100	-1.00103800	0.66159500
O	-2.79899000	0.03901500	2.06027600
Br	-2.93485500	-2.04603100	-0.78674900
C	5.35070700	-0.45377900	-0.64329700
C	4.78941900	-0.46613200	0.64322800
C	3.40271900	-0.49067000	0.75488400
C	2.53733600	-0.49699700	-0.39495700
C	3.13121400	-0.47660200	-1.67159500
C	4.52564800	-0.45706200	-1.78313700
H	6.43181500	-0.43664100	-0.75584300
H	5.42195200	-0.45869500	1.52831000
H	2.51140300	-0.47490300	-2.56588800
H	4.98104800	-0.44332000	-2.77115500
C	1.20043500	-0.51519800	0.11019700
C	1.26726100	-0.52601900	1.49356900
N	2.59609800	-0.49551000	1.89258600
H	2.91866000	-0.55244600	2.84872600
O	0.22289700	-0.54635200	2.26679200
H	-0.24974500	-1.21137500	-1.28575000
H	-1.07062200	-1.97490200	1.11730200

9
E = -3472.011501
G = -3471.764084

C	1.71853800	0.21210300	-1.03500300
C	2.16772000	-1.29417000	-1.15865500
C	3.87349900	-0.36807800	0.03151300
C	2.86843500	0.83671500	-0.15390100
H	1.66921500	0.66795200	-2.02568200
H	3.35549100	1.70539200	-0.60459000
C	2.85396800	-1.53350300	0.21911900
H	3.34321100	-2.50968600	0.27326100
H	2.17908800	-1.38487000	1.06591500
C	3.40455100	-1.24489200	-2.06796900
H	3.40460000	-1.51260400	-3.11675600
C	4.40744400	-0.69208300	-1.36610700
H	5.39096300	-0.41871900	-1.72603900
H	1.37138100	-1.97775700	-1.44703300
H	4.59530700	-0.19426800	0.82738300
C	2.35554800	1.15927000	1.23599600
C	0.38093200	0.47441200	-0.26057800
C	0.83969000	1.00937700	1.10249000

H	4.66813500	2.33945700	0.13319900
C	1.05426500	-0.76335400	-0.44682300
C	1.28174900	-2.21407000	-0.45670200
N	2.59257700	-2.43576800	-0.06289600
H	3.01613000	-3.35420600	-0.05986400
O	0.49315700	-3.13618300	-0.76348800
H	-0.65901400	-0.94446100	-1.74243400
H	-0.74585500	-1.91948000	0.79127800

6
E = -3472.030174
G = -3471.787116

C	0.93764300	0.91403200	1.28580500
C	0.24998900	2.27200300	1.67967800
C	0.86837600	2.60463300	-0.49409100
C	1.37468100	1.15042400	-0.19367000
H	1.81103900	0.74682100	1.92418200
H	2.45994200	1.06087300	-0.30766200
C	-0.44661300	2.66542400	0.34798300
H	-0.85482800	3.67921100	0.38460900
H	-1.20978600	1.95870100	0.04100200
C	1.40747000	3.29231500	1.66978200
H	1.88540700	3.68554100	2.55732100
C	1.76808900	3.49050700	0.39273400
H	2.60119600	4.07480600	0.02477900
H	-0.36339500	2.23604200	2.57872900
H	0.81006500	2.85871500	-1.55138100
C	0.80568600	-0.01916300	-1.00851800
C	0.18585800	-0.41872700	1.28999800
C	0.34825300	-1.11085000	-0.03863000
O	0.70405600	-0.05576900	-2.23701100
Br	3.84981900	-1.47956300	-0.55599900
C	-4.77691800	0.35427600	-1.29240900
C	-4.67820500	-0.59589200	-0.26821500
C	-3.41427700	-0.91762200	0.20906500
C	-2.24273100	-0.27998100	-0.27332000
C	-2.35587000	0.59422300	-1.35264000
C	-3.62760700	0.92353400	-1.84599000
H	-5.75379500	0.62240700	-1.67701600
H	-5.56118200	-1.08561300	0.12286300
H	-1.47551900	0.99198400	-1.83617000
H	-3.71292900	1.61581700	-2.67483300
C	-1.08344800	-0.88930400	0.44935800
C	-1.68649800	-2.04161200	1.25006500
N	-3.06123700	-1.91979800	1.12444800
H	-3.71723600	-2.54402000	1.58182200
O	-1.08062100	-2.87725100	1.93194100
H	0.26133100	-1.02336000	2.18571300
H	0.71394300	-2.11982200	-0.16647400

TS-(1+7)
E = -3794.950949

C	1.61461300	-1.18373600	-0.87791300
C	1.94103400	-2.23039200	0.25196700
C	3.68422500	-0.79797800	0.40910600
C	2.84253600	-0.21565000	-0.77569200
H	1.56786100	-1.69286100	-1.84687200
H	3.43742700	-0.20673500	-1.69763600
C	2.55789100	-1.31203000	1.33870900
H	2.93944400	-1.87382800	2.19817100
H	1.88780500	-0.51883700	1.68661700
C	3.19235600	-2.96841400	-0.21881500
H	3.19197600	-3.96506900	-0.65121600
C	4.23038700	-2.12188200	-0.11577300
H	5.25151500	-2.28517700	-0.44924700
H	1.11115100	-2.87991800	0.53653300
H	4.41112900	-0.10087800	0.83241800
C	2.25799400	1.19053500	-0.61345400
C	0.36824900	-0.26624300	-0.78152200
C	0.85783300	1.05973300	-0.71656300
O	2.96753500	2.22414300	-0.52488800
Br	-0.29166600	2.57262200	-0.94451700
C	-4.65789900	-1.61854600	-0.93348800
C	-4.39388500	-0.50312600	-0.12639800
C	-3.11095200	-0.38454200	0.40353200
C	-2.08674300	-1.32861100	0.14884500
C	-2.37011600	-2.42758600	-0.66845800

O	3.03664000	1.40119800	2.26504400
Br	-2.27056900	3.58252300	-0.67095600
C	-3.40018600	-3.69665900	-0.31629600
C	-3.07017000	-3.15181100	0.92637500
C	-2.11255600	-2.14200200	0.96729900
C	-1.45692000	-1.66601900	-0.22977600
C	-1.81309400	-2.23645100	-1.46287900
C	-2.77924200	-3.24075800	-1.49555100
H	-4.14658800	-4.48028500	-0.37211800
H	-3.55013900	-3.50233100	1.83211000
H	-1.34074400	-1.89501800	-2.37693400
H	-3.05914400	-3.68149800	-2.44582600
C	-0.52244000	-0.65864400	0.19696300
C	-0.67220300	-0.55054600	1.55628900
N	-1.60680900	-1.41811700	2.06131900
H	-1.87178500	-1.53152400	3.03212700
O	0.06401700	0.43474600	2.19790300
H	-0.19669200	1.24237500	-0.78939900
H	0.50705800	2.02626100	1.08825600

7

E = -761.575288

G = -761.488671

C	-2.94623100	-0.77448300	-0.00057800
C	-1.71243700	-1.43516500	-0.00053900
C	-0.55364600	-0.65411000	-0.00023200
C	-0.59201600	0.77625200	-0.00005000
C	-1.85031700	1.41161700	-0.00009400
C	-3.01107100	0.63469600	-0.00038200
H	-3.86483600	-1.35616800	-0.00072100
H	-1.65834900	-2.52151000	-0.00056000
H	-1.91734800	2.49785800	-0.00008700
H	-3.98300500	1.12328100	-0.00052900
C	0.76909600	1.22779600	-0.00033400
H	1.11146300	2.25494500	-0.00078300
C	1.60146400	0.11075400	0.00035900
N	0.77878400	-1.01744800	0.00025400
H	1.13639100	-1.96273600	0.00089000
S	3.34344700	-0.04360500	0.00069400

Intermediate-(1+7)

E = -3794.997132

G = -3794.756340

C	-0.99212300	1.33790900	-0.74257600
C	-1.02718300	2.35886000	0.45501500
C	-3.22050400	1.91445800	0.13674600
C	-2.50139700	0.97923000	-0.91632800
H	-0.58071100	1.83896000	-1.62243500
H	-2.90585400	1.13545100	-1.92180800
C	-2.21186200	1.84179700	1.30751500
H	-2.46976100	2.52743100	2.12098400
H	-2.05884300	0.84220400	1.72397100
C	-1.67010000	3.60831000	-0.14107500
H	-1.12636900	4.49589000	-0.45227100
C	-2.97190000	3.33924900	-0.34243000
H	-3.70719000	3.95904200	-0.84714200
H	-0.06660800	2.49543000	0.95434500
H	-4.25786700	1.63506100	0.33342400
C	-2.62978000	-0.49716600	-0.57143000
C	-0.23038600	-0.03079900	-0.57441500
C	-1.28987500	-1.01123900	-0.06062900
O	-3.65173600	-1.15434200	-0.67925400
C	5.02779000	0.84000600	-1.09268300
C	4.69839400	0.48732900	0.22066500
C	3.35515000	0.23176500	0.50910100
C	2.32749600	0.32187400	-0.47639500
C	2.69011700	0.67907000	-1.79060200
C	4.03168300	0.93303200	-2.08654000
H	6.06459600	1.04471900	-1.34826500
H	5.46302900	0.41230900	0.99057900
H	1.93745000	0.76189800	-2.57196300
H	4.31362300	1.20870200	-3.10030600
C	1.07867200	-0.00582100	0.16458000
C	1.36235600	-0.28965200	1.50605000
N	2.73924700	-0.13453800	1.68579600
H	3.19531500	-0.29396600	2.57344800
H	-0.00785200	-0.33797900	-1.60583500

C	-3.66049300	-2.57024400	-1.19903400
H	-5.65026400	-1.74516300	-1.35849300
H	-5.16332300	0.23598900	0.08034700
H	-1.60371200	-3.16744200	-0.88776000
H	-3.89108000	-3.42775500	-1.82614600
C	-0.85880700	-0.82957700	0.78056400
C	-1.27071500	0.32206300	1.56588300
N	-2.57675900	0.59360500	1.24220800
H	-3.08796900	1.37809400	1.62617500
H	-0.44198600	-0.49208300	-1.46937800
H	-0.15444000	-1.50604900	1.24082700
S	-0.38282800	1.21093400	2.70740300

8

E = -3795.018440

G = -3794.777815

C	-1.28883200	0.76614200	0.51886600
C	-1.05436900	0.02665400	1.88811500
C	-3.25360900	-0.34222200	1.51929200
C	-2.80069300	0.48877300	0.25260500
H	-1.08110000	1.83162600	0.63598300
H	-3.41615200	1.38804500	0.13968800
C	-1.98727700	-1.20100200	1.74852300
H	-2.04477100	-1.79520000	2.66613900
H	-1.73776400	-1.85867600	0.90821200
C	-1.83772000	0.83338700	2.91802700
H	-1.39591900	1.53843600	3.61638200
C	-3.14592600	0.61798800	2.69638800
H	-3.98949200	1.10811900	3.17351900
H	-0.00534800	-0.16116100	2.11893400
H	-4.20742000	-0.85677700	1.38616900
C	-2.89073900	-0.30613700	-1.03757200
C	-0.48416100	0.26039700	-0.73786500
C	-1.51397500	-0.43448900	-1.68714900
O	-3.91787600	-0.76542100	-1.51208000
Br	1.22239600	3.48964200	-0.87808300
C	4.33924400	-1.60296600	1.27063500
C	3.60789500	-2.53316500	0.52979500
C	2.38780700	-2.11535900	-0.00934800
C	1.88584800	-0.78678100	1.67588000
C	2.65469200	0.13120400	0.90932200
C	3.86626300	-0.28576700	1.45697600
H	5.29022200	-1.89836900	1.70645200
H	3.97159000	-3.54684500	0.38201400
H	2.30492600	1.15109600	1.04339700
H	4.46319200	0.41658500	2.03379900
C	0.61682300	-0.73485300	-0.50573900
C	0.41907900	-1.97625900	-1.05332800
N	1.46158200	-2.82454000	-0.76725700
H	1.56216300	-3.77991700	-1.08066000
H	-0.09009900	1.15376900	-1.23158500
S	-1.05403900	-2.23733700	-1.98078200
H	-1.55342100	0.03104500	-2.67639700

TS-XVIIIb

E = -3794.979966

G = -3794.738552

C	-0.80201000	0.89036500	-0.95062700
C	0.01096100	2.21539600	-0.73420600
C	-1.87645400	2.61456200	0.44479000
C	-2.10764000	1.16958000	-0.13496200
H	-1.01726800	0.75606500	-2.01341900
H	-3.01344600	1.15069900	-0.74901600
C	-0.35600600	2.57778700	0.72613800
H	0.03623800	3.55568500	1.02564300
H	-0.06422100	1.82355700	1.46067900
C	-0.77629400	3.29408700	-1.47545500
H	-0.50980300	3.69714000	-2.44861500
C	-1.89889300	3.53186500	-0.77535400
H	-2.73502200	4.16465100	-1.05941500
H	1.07127500	2.13676200	-0.98129700
H	-2.54467900	2.87533000	1.26862700
C	-2.25089500	0.03847900	0.88006600
C	-0.17887300	-0.46412900	-0.40838000
C	-1.21551200	-1.00236100	0.56257000
O	-3.09218700	-0.02360100	1.76621200

H	-1.28752900	-1.06717400	1.03512000
Br	-0.95624600	-2.87401600	-0.61948800
S	0.37769100	-0.75751200	2.87664400

10
E = -3794.985075
G = -3794.747430

C	0.99788400	0.53477700	1.24032500
C	0.57015200	1.81918500	2.02819900
C	1.06787700	2.61609500	-0.03745100
C	1.38945500	1.08307200	-0.15766800
H	1.86232500	0.07613100	1.73321300
H	2.45671900	0.93483200	-0.35995400
C	-0.14590500	2.63281100	0.93004000
H	-0.39572800	3.64795900	1.25496800
H	-1.04421500	2.14993300	0.55552500
C	1.85384800	2.64634800	2.14952600
H	2.45731400	2.72635700	3.04900300
C	2.14541700	3.12410700	0.92795400
H	3.03851400	3.66250500	0.62444600
H	0.02428200	1.62939400	2.95542600
H	0.97548200	3.14996400	-0.98597800
C	0.72129500	0.16491800	-1.17978900
C	0.07212000	-0.66238200	0.98618800
C	0.11553600	-1.03415800	-0.45935700
O	0.74612400	0.30072400	-2.39220900
Br	4.18274200	-1.15638400	-0.69185000
C	-4.75576600	1.33763200	-1.12262500
C	-4.78770700	0.15464800	-0.37683800
C	-3.56606300	-0.41892500	-0.03878600
C	-2.32009000	0.14923200	-0.36349600
C	-2.31726900	1.29227500	-1.16698000
C	-3.53415100	1.88530700	-1.53185800
H	-5.68815500	1.81519000	-1.41017300
H	-5.72646200	-0.31453600	-0.09697500
H	-1.39569300	1.72946900	-1.53120700
H	-3.52255700	2.77968400	-2.14815700
C	-1.26261600	-0.78588800	0.15192900
C	-2.04199600	-1.99898600	0.62666900
N	-3.34677800	-1.65873200	0.57543700
H	-4.08382200	-2.29923700	0.84733800
H	0.11019300	-1.44752900	1.73385100
S	-1.47102700	-3.48579200	1.14477600
H	0.31861000	-2.02906500	-0.84925400

TS-XIXb
E = -3794.953795
G = -3794.712777

C	-0.97221600	1.13676400	-1.00635600
C	-0.13684900	2.45925600	-1.16130300
C	-1.42755800	2.92952300	0.64098400
C	-1.78648400	1.45188400	0.30055600
H	-1.63807800	1.04549700	-1.86637400
H	-2.86343500	1.32249700	0.16504300
C	0.07628900	2.90219800	0.31591000
H	0.55848900	3.88199300	0.39656200
H	0.61551600	2.18224000	0.93780800
C	-1.16855200	3.50691100	-1.58487800
H	-1.30021300	3.85995800	-2.60359400
C	-1.94369500	3.77308300	-0.52077600
H	-2.83303300	4.39569400	-0.49004800
H	0.73526900	2.37638500	-1.81200000
H	-1.72122600	3.24191000	1.64529400
C	-1.33677000	0.38697500	1.29699700
C	-0.33732400	-0.29431300	-0.82888700
C	-0.81536600	-0.75915700	0.49771300
O	-1.42221400	0.43631500	2.51910600
Br	-3.34298000	-1.57157900	0.16511400
C	5.05406400	0.60847700	0.61028000
C	4.62946700	-0.72031500	0.56557600
C	3.30612000	-0.96894800	0.20643500
C	2.34729400	0.04860100	-0.07857100
C	2.83623200	1.37162800	-0.07496500
C	4.16307400	1.63841100	0.27170300
H	6.08040500	0.84039800	0.88139400
H	5.30923700	-1.54095900	0.77883500
H	2.21614000	2.20288300	-0.36464600

Br	-2.74238800	-2.09547200	-1.03944000
C	5.23147100	-0.36606300	-1.04437200
C	4.83754700	-0.38484400	0.29729800
C	3.46896900	-0.41714900	0.57380900
C	2.47945100	-0.41747700	-0.45891900
C	2.90726000	-0.39469700	-1.80066700
C	4.27458600	-0.37146000	-2.08073400
H	6.29026300	-0.34381000	-1.28984800
H	5.57308900	-0.37885200	1.09829900
H	2.18179800	-0.39174600	-2.61134300
H	4.60950600	-0.35506100	-3.11529900
C	1.20066800	-0.43375600	0.19397400
C	1.43023500	-0.45496600	1.55809200
N	2.79820600	-0.43838500	1.78555800
H	3.22821500	-0.46992700	2.69946100
H	-0.12725400	-1.15359900	-1.25634000
S	0.19035200	-0.51662500	2.77649500
H	-1.16212000	-1.95318800	1.06139200

H	4.50845200	2.66895100	0.26669100	
C	1.09502400	-0.63833600	-0.41932900	
C	1.41676500	-2.06141500	-0.42438900	
N	2.70568700	-2.19816900	0.00903200	
H	3.17511300	-3.09320800	0.05682400	
H	-0.62775100	-0.93485400	-1.66627700	
S	0.49331400	-3.40192600	-0.92910100	
H	-0.66281800	-1.74399200	0.90483100	